

SIC Codes for 40 Industries

#	INDUSTRY	Standard Industrial Classification (SIC) Code(s)
1	Adhesives and Sealants Manufacture	2891
2	Auto and Other Laundries	7211, 7213-7219, 7542
3	Can (metal) Manufacture	3411
4	Dyes and Pigments Manufacture	2865
5	Electronic Components Manufacture	3674, 3679
6	Electroplating	3471
7	Foundries	332, 336
8	Ink Formulation	2983
9	Inorganic Chemicals Manufacture	281
10	Large Household Appliances and Parts Manufacture	3631-3633, 3639, 3431, 3469
11	Leather Tanning and Finishing	3111
12	Lubricant Manufacture	2911, 2992
13	Manufacture of Photographic Equipment and Supplies, Photographic Processing	7221, 7333, 7395, 7819
14	Metal Finishing	3411-62, 3465-71, 3482-3599, 3613-23, 3629, 3634-6, 3643-51, 3661-71, 3673, 3676-8, 3693-4, 3699, 3711-3841, 3851, 3873-999
15	Motor Vehicle Manufacture	3711, 3713
16	Organic Chemicals Manufacture	2865, 2869
17	Ore Mining and Dressing	101-109
18	Paint Formulation	2851
19	Paper and Paperboard Mills	2621, 2631, 2661
20	Paper Mills except Building Paper Mills	2621
21	Paper Board Mills	2631
22	Building Paper and Board Mills	2661
23	Pesticides Manufacture	2819, 2869, 2879
24	Petroleum Refining	2911
25	Plastic Products Manufacture	3079
26	Plastic Resins and Synthetic Fabrics	2821, 2823, 2824
27	POTWs (Industrial)	4952
28	POTWs (All Facilities)	4952
29	Primary Metal Forming Manufacture	3315-17, 3351-57, 3463, 3497
30	Printing	271-277
31	Pulp Mills	2611
32	Rubber Products Manufacture	3011, 3021, 3031, 3041
33	Soaps, Detergents, etc. Manufacture	2841-44
34	Steam Electric Power Plants	4911
35	Textile Dyeing and Finishing (Carpets)	2271-72, 2279
36	Textile Dyeing and Finishing (Knit Goods)	225, 2292
37	Textile Dyeing and Finishing (Wool Goods)	2231
38	Textile Dyeing and Finishing (Woven Goods)	2261-62, 2269
39	Textile Dyeing and Finishing (Knit, Wool, and Woven Goods)	2231, 2250, 2269, 2292
40	Yarn and Thread Mills	2281-84

Glossary of Useful Terms

7Q10 flow: Lowest 7-consecutive day average stream flow over a 10 year period (used to assess chronic risks to aquatic life).

Acute toxicity: Adverse effects on any living organism that results from a single dose or single exposure of a chemical; any poisonous effect produced within a short period of time, usually less than 96 hours.

ADD (Average daily dose): The estimate of dose averaged over the number of years of use/exposure to the chemical; used in assessments of risk of non-cancer chronic health effects.

APDR (Acute potential dose rate): The estimated dose on a given day; used in assessments of the risk of acute toxic effects.

BCF: Bioconcentration factor (BCF) is the ratio (in L/kg) of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water. BCF indicates the potential for the chemical to concentrate in lipids (fats) of organisms.

Bioaccumulation: Process in which lipid soluble chemicals are stored in fatty tissue (lipids) of organisms and can increase in concentration over time.

Bioassay: Testing method that measures the effects of a material on living organisms.

Bioconcentration: Bioaccumulation of lipid soluble chemicals in fatty tissues (lipids) of organisms at concentrations higher than that of the surrounding water.

Biodegradable: Ability of a substance to be broken down physically and/or chemically by microorganisms.

Biomagnification: Process in which lipid soluble substances increase in fatty tissues (lipids) of organisms higher in the food web as contaminated food species are consumed.

Carcinogen(ic): Ability of a substance to cause cancer.

Chemical Abstract Service (CAS): Organization which assigns unique numbers to chemical substances submitted to them. CAS Registry Numbers are the unique identifier for a chemical substance, while chemical names may not be unique.

Chemical class: The general chemical group to which a chemical belongs (e.g., acid, base, hydrocarbon, etc.).

Chronic Toxicity: Adverse effects on any living organism in which symptoms develop slowly over a period of time (often the life time of the organism) or reoccur frequently.

Concern concentration (CC) or Concentration of Concern (COC): Reported in parts per billion (ppb) or parts per million (ppm), provides the concentration of a chemical in a stream and indicates the concentration at which harm is more likely to occur to aquatic organisms. CC is determined by dividing the lowest chronic toxicity value by 10.

Direct discharge: Under NPDES permitting, the discharge of chemicals or compounds directly to a surface water body.

Dose: In terms of monitoring exposure levels, the amount of a toxic substance taken into the body over a given period of time.

Dose Response: The manner in which an organism's response to a toxic substance changes as its overall exposure to the substance changes.

EC50 (Effective Concentration 50): Median effective concentration is the concentration of a pollutant at which 50% of the test organisms die; a common measure of acute toxicity.

Glossary of Useful Terms (continued)

Effluent: The stream flowing out of a facility or water body. The concentrations in it's flow are used to estimate potential health effects of the discharge.

Exposure: Pollutants that come in contact with the body and present a potential health threat, via inhalation, ingestion, or dermal routes. The route, magnitude, and duration of exposure contributes to the ultimate risk for the organism.

Half-life: Time required for one-half of a chemical or compound to degrade.

Harmonic mean: The number of daily flow measurements divided by the sum of the reciprocals of the flows. A value that is more conservative than the arithmetic mean flow value. Used to assess chronic risks to humans.

Hazard: Potential for a substance to cause adverse effects to organisms, for example birth defects.

High end: A plausible estimate of an individual exposure or dose for those persons at the upper end of an exposure or dose distribution, above the 90th percentile, but no higher than the individual in the population who has the highest exposure.

Hydrophilic: Having an affinity for, or capable of dissolving in, water.

Influent: Stream flowing into a facility or water body.

Indirect discharge: Under NPDES permitting, unlike a direct discharger, an indirect discharger from a nonresidential source pumps effluent to another facility that has a permit to discharge to the stream. Indirect dischargers often pretreat their discharges prior to pumping them to the publicly owned treatment works.

KOC: Organic carbon partition coefficient - the ratio of amount of a chemical adsorbed per unit weight of organic carbon to the chemical concentration in solution at equilibrium. Is an indication of how the chemical will partition itself between the solid and solution phases of a water-saturated or unsaturated soil.

KOW: Octanol-water partition coefficient - the ratio of a chemical's concentration in the octanol phase to it's concentration in the aqueous phase of a two-phase octanol/water system.

LADD (Lifetime average daily dose): The estimated dose to an individual averaged over a lifetime of 70 years; used in assessments of *carcinogenic* risk.

LC50 (Lethal Concentration 50): Median lethal concentration is the concentration of a pollutant at which 50% of the test organisms die; a common measure of acute toxicity.

LD50 (Lethal Dose 50): The dose of a toxicant that will kill 50% of test organisms within a designated period of time. The lower the LD50, the more toxic the compound.

Lipophilic: Having an affinity for, or capable of dissolving in, fat and fatty materials.

Loading: The amount of chemical that is discharged to a stream after treatment, reported in kg/day.

Milligrams/liter (mg/L): A measure of concentration used in the measurement of fluids that is roughly equivalent to parts per million.

Moiety(ies): Compounds formed when a larger compound is subdivided.

MSDS (Material Safety Data Sheet): Printed material concerning a hazardous chemical including its physical properties, hazards to personnel, fire and explosive potential safe handling and transportation recommendations, health effects, reactivity, and proper disposal. Originally established for employee safety by OSHA.

Mutagenicity: The property of a chemical to cause genetic mutations that are expressed in the next generation but not necessarily in the organism exposed to the mutagen.

Glossary of Useful Terms (continued)

No Observed Adverse Effect Level (NOAEL) or No Observed Effect Level (NOEL): Level of exposure which does not cause observable harm.

NPDES (National Pollutant Discharge Elimination System): is the primary permitting program under the Clean Water Act which requires that dischargers of chemicals to surface waters obtain a permit from EPA. A NPDES permit number is a nine-character number with the two letter State abbreviation beginning the number (e.g., NC0001234).

Parts per billion (ppb): One ppb is comparable to one kernel of corn in a filled, 45-foot silo, 16 feet in diameter.

Parts per million(ppm): One ppm is comparable to one drop in the gasoline tank of a full-size car.

Parts per trillion (ppt): One ppt is comparable to one drop in a swimming pool the size of a football field and 43 feet deep.

Permissible Exposure Limit (PEL): Workplace exposure limits for contaminants established by OSHA.

Point Source: A stationary location or fixed facility such as an industry or municipality that discharges pollutants into air or surface water.

Pollution: Any substances in environmental media that degrade the natural quality of the environment.

Pollution Prevention (P2): The concept stating that it is easier to prevent pollution than to clean up pollution after it has occurred.

Potential Dose Rate(s) PDR(s): Provide an estimate of possible exposure rate to receptor from expected use, usually derived by modeling using default exposure factors.

POTW (Publicly Owned Treatment Works): A municipal or public service district sewage treatment system.

Reach: A reach is a stream or river segment identified by EPA and assigned an 11-digit ID number. The first two numbers indicate the hydrologic region of the United States in which the reach is located.

Reference Dose (RfD): The concentration of a chemical that is known to cause health problems.

Release: Any spilling, leaking, pumping, pouring, emitting, emptying, discharging, injecting, escaping, leaching, dumping, or disposing into the environment of a hazardous or toxic chemical.

Risk: A measure of the chance that damage to life, health, property, or the environment will occur.

Risk Assessment: A process to determine the increased risk from exposure to environmental pollutants together with an estimate of the severity of impact. Risk assessments use specific chemical information plus risk factors.

SARs: Structure Activity Relationship (SAR) predict the toxicity of chemicals based on their structural similarity to chemicals for which toxicity data are available. SARs express the correlations between a compound's physicochemical properties and its toxicity. SARs measured for one compound can be used to predict the toxicity of similar compounds belonging to the same chemical class. EPA routinely uses to estimate toxicity of chemicals submitted as Pre-Manufacture Notices mandated by Section 5 of the Toxic Substances Control Act (TSCA).

SIC Code: Standard Industrial Classification Code system is a four digit number that identifies the specific industrial activity. For a complete listing of SIC codes, see Standard Industrial Classification Manual. 1987. Supt. of Documents, U.S. Government Printing Office, Washington, DC.

Toxicity Testing: Biological testing (usually with an invertebrate, fish, or small mammal) to determine the adverse effects, if any, of a chemical substance.

APPENDIX A

Case Studies

Case Study A - Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Uses the Models ECOSAR and the E-FAST General Population Exposure from Industrial Releases Module

Case Study B - Consumer Dermal Exposure

Uses the E-FAST Consumer Exposure Pathway (CEM) Module

Case Study C – Workplace Releases and Exposures

Uses ChemSTEER - the Chemical Screening Tool for Exposures and Environmental Releases

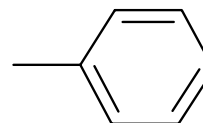
CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Introduction

The purpose of this case study is to determine the aquatic toxicity of Chemical A and to assess potential aquatic impacts and human exposures that may occur as a result of *effluent* discharges from the manufacturing facility (Company ABCDE) in Smalltown, New York. The following models will be used to accomplish this task: ECOSAR and E-FAST: General Population Exposure from Industrial Releases module.

- ECOSAR will be used first to estimate a *concern concentration* for the chemical.
- E-FAST will then be used to estimate the surface water concentration and the likelihood of potential impacts.

Chemical A (structure at right) is a compound in the neutral organic chemical class. No significant aquatic toxicity testing has been done on Chemical A.



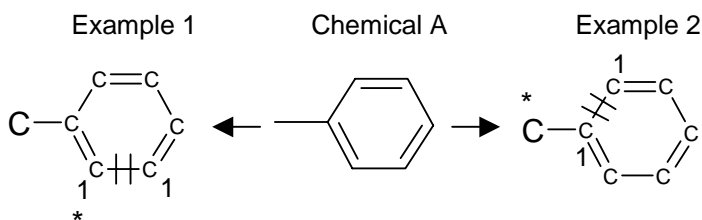
Step 1. Toxicity Determination

Because no aquatic toxicity data are available for Chemical A, ECOSAR will be used to predict its aquatic toxicity based on structural similarities to other neutral organic chemicals. The following physical/chemical properties will be assumed for Chemical A that are inputs to run the ECOSAR and E-FAST models:

- measured water solubility = 573.1 mg/L;
- melting point = 25° C;
- log KOW = 2.540 (ClogP);
- measured log KOW = 2.730; and
- fish BCF = 175 (not log BCF).

Running ECOSAR

Since you have no CAS Number for Chemical A, you will need to write SMILES notation to run ECOSAR. For help in writing SMILES see Appendix C or the Help screen in ECOSAR. There are many correct ways to write SMILES for a given chemical. Two examples are given below. Start the SMILES string at the “*”.



Example 1 SMILES = c1c(C)cccc1

Example 2 SMILES = Cc1ccccc1

Open ECOSAR and select “All Others” Chemicals group. Enter measured data and SMILES notation (Figure A1), then click on Calculate button. Figure A2 presents the results of running the model.

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Figure A1
ECOSAR Data Entry Screen

SMILES : c(cccc1)(c1)C
CHEM : Benzene, methyl-
CAS Num: 000108-88-3
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H8
MOL WT : 92.14
Log Kow: 2.54 (User entered)
Melt Pt: 25.00 deg C
Wat Sol: 573.1 mg/L (measured)

ECOSAR v0.99g Class(es) Found

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics				
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	41.891
Neutral Organics	: Fish	96-hr	LC50	21.225
Neutral Organics	: Fish	14-day	LC50	41.891
Neutral Organics	: Daphnid	48-hr	LC50	23.608
Neutral Organics	: Green Algae	96-hr	EC50	15.225
Neutral Organics	: Fish	30-day	ChV	2.983
Neutral Organics	: Daphnid	16-day	EC50	1.533
Neutral Organics	: Green Algae	96-hr	ChV	2.080
Neutral Organics	: Fish (SW)	96-hr	LC50	6.313
Neutral Organics	: Mysid Shrimp	96-hr	LC50	4.163
Neutral Organics	: Earthworm	14-day	LC50	386.488

Note* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: 5.0
Green algal EC50 toxicity log Kow cutoff: 6.4
Chronic toxicity log Kow cutoff: 8.0
MW cutoff: 1000

Inputs:

❖ SMILES	
❖ Chemical Name	
❖ Data	
Log Kow (ClogP)	2.540
Meas. WS	573.1
Meas. MP	25.0
Meas. Log Kow	2.730

Figure A2
Results of Running
ECOSAR

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Figure A2
Results of Running ECOSAR

Inputs: SMILES Chemical Name Log Kow (ClogP) 2.540 Meas. WS 573.1 Melting Pt 25.0 Meas. Log Kow 2.730				
SMILES : c(ccccl)(cl)C CHEM : Benzene, methyl- CAS Num: 000108-88-3 ChemID1: ChemID2: ChemID3: MOL FOR: C7 H8 MOL WT : 92.14 Log Kow: 2.54 (User entered) Melt Pt: 25.00 deg C Wat Sol: 573.1 mg/L (measured)				
ECOSAR v0.99g Class(es) Found Neutral Organics				
ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
=====	=====	=====	=====	=====
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	41.891
Neutral Organics	: Fish	96-hr	LC50	21.225
Neutral Organics	: Fish	14-day	LC50	41.891
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Neutral Organics	: Green Algae	96-hr	ChV	2.080
Neutral Organics	: Fish (SW)	96-hr	LC50	6.313
Neutral Organics	: Mysid Shrimp	96-hr	LC50	4.163
				mg/kg (ppm) dry wt soil
				=====
Neutral Organics	: Earthworm	14-day	LC50	386.488
Note* = asterick designates: Chemical may not be soluble enough to measure this predicted effect. Fish and daphnid acute toxicity log Kow cutoff: 5.0 Green algal EC50 toxicity log Kow cutoff: 6.4 Chronic toxicity log Kow cutoff: 8.0 MW cutoff: 1000				

Note: The standard toxicity profile used by EPA for freshwater species is:

Acute Effects: Fish 96-hr LC50 (mg/L)
Daphnid 48-hr LC50
Green algal 96-hr EC50
Chronic Effects: Fish ChV
Daphnid ChV or 16d EC50
Green algal ChV

Chemical A Aquatic Toxicity Profile is:

Acute Effects:	Fish	96-hr LC50	22.0
	Daphnid	48-hr LC50	24.0
	Green algal	96-hr EC50	15.0
Chronic Effects:	Fish	ChV	3.0
	Daphnid	ChV	1.5
	Green algal	ChV	2.0

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Determine Concern Concentration

The next step is translating the predicted endpoints into a freshwater (FW) concern concentration (CC). The following equation is used to calculate the FW CC. The lowest chronic value, the predicted endpoint for Daphnid (1.5 mg/L or ppm), was used. An uncertainty factor (assessment or safety factor) is 10 was used to account for the uncertainty of laboratory to field variation, and as a margin of safety.

$$\begin{aligned} & (\text{Predicted Endpoint} \times 1,000 \text{ conversion from ppm to ppb}) / \text{safety factor} \\ & (1.5 \text{ ppm} \times 1,000) / 10 = 150 \text{ ppb, rounded up to 200 ppb.}^* \end{aligned}$$

*Note: The CC is rounded up to one significant digit to be conservative, and because the safety factor is one significant digit.

Step 2. Estimation Of Surface Water Concentrations

Now that a freshwater CC for Chemical A (200 ppb) has been established, the site-specific release can be evaluated. Assume the following:

- Company ABCDE will discharge 200 kg/day of Chemical A for 300 days per year; and
- There will be 50 percent removal of Chemical A in wastewater treatment.
- The fish BCF value predicted by EPI Suite™ is 175 (not the log BCF)

After talking to Company representatives, the assessor has determined that:

- Company ABCDE discharges to the Little Genesee Creek;
- The NPDES Number is NY0022381.

Using this information the assessor can use the E-FAST model to calculate: the concentration of Chemical A in the Little Genesee Creek; the potential drinking water exposures; and the potential fish ingestion exposure and the potential risk to the aquatic environment.

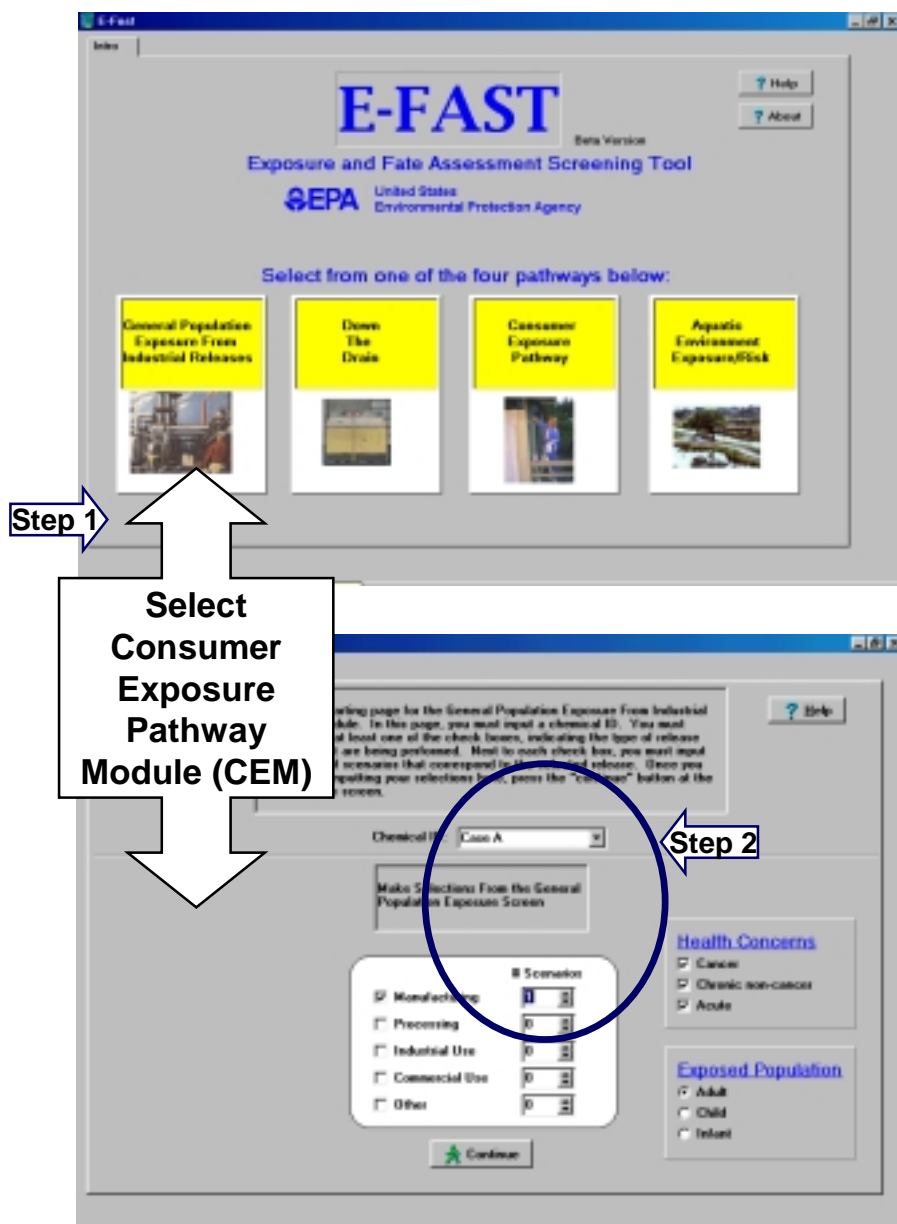
CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module

The following is a step-by-step description of how to run the CEM module.

Once you have entered the E-FAST model:

1. Select: General Population Exposure Module;
2. Enter the chemical identification "Case A", and select 1 Manufacturing Scenario, then click on Continue button.



CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

3. You automatically go to the Release Info page. Put a check in the Surface Water box and add Release Amount (200 kg/site/day) and Release Days per Year (300 days/yr)
4. Click on Facility button. You go to the Select a Facility screen.

E-Fast

Intro | General Pop Exp | **Release Info** | PChem | Exp Factors | Fate

General Release Info | Select a facility | ? Help

Chemicals ID/Rel #
Case A.1

Release Activity
Manufacture

Sites **1**

Select the desired releases and input the amount of release and number of days/year of release if needed

	Release	# Days per year of Release
<input checked="" type="checkbox"/> Surface water	200 kg/site/day	300 days/yr
Choose facility or SIC code analysis:		
<input checked="" type="radio"/> Facility	NPDES #: NY0022381	
<input type="radio"/> SIC Code	Description:	
<input type="checkbox"/> Landfills (including sludge)		
Landfill	0.00 kg/yr	
Sludge	0.00 kg/yr	
<input type="checkbox"/> Ambient air from fugitive releases		
Ambient air from fugitive releases	0.00 kg/site/day	0 days/yr

Continue

Step 4 (points to Continue button)

Step 3 (points to Surface water section)

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

5. In the Select a Facility screen, type the *NPDES* number (NY0022381) in the proper box. Click on Perform Search for Facility Button. When the search finds the facility, Double click the facility name. Click on Continue button.

The screenshot shows the 'E-Fast' software window with the 'General Release Info' tab selected. The 'Select a facility' sub-tab is active. The 'Release Information - Facility Selection Screen' is displayed. The 'Locate facilities where this field' dropdown is set to 'NPDES', and the 'has the following substring:' text box contains 'NY0022381'. The 'Perform search for facilities' button is highlighted. Below the search area, a table lists the search results:

NPDES	FACILITY NAME	LOCATION	REACH	REACH NAME
NY0022381	BOLIVAR (V) WWTF	BOLIVAR NY 14715	05010001025	LITTLE GENES

The 'BOLIVAR (V) WWTF' facility name is circled, and a blue arrow labeled 'Step 5' points to it. Another blue arrow labeled 'Step 5' points to the 'Perform search for facilities' button.

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

6. You are sent to the Physical Chemical Properties screen, and you should enter the *BCF* (175) and *Concern Concentration* (200 ppb or µg/L). Click on Continue button.

The screenshot shows the E-FAST software interface. The title bar reads 'E-FAST'. The menu bar includes 'Intro', 'General Pop Exp', 'Release Info', 'PChem', 'Exp Factors', and 'File'. The 'PChem' tab is selected. A 'Help' button with a question mark icon is in the top right. The main window is titled 'Physical Chemical Properties'. Inside, 'Chemical ID: Case A' is displayed. Below this, there are two input fields: 'Bioconcentration Factor' with the value '175' and 'Concentration of concern' with the value '200' and the unit 'ug/L'. There are two radio buttons: 'High end PDM analysis' (which is selected) and 'Average PDM analysis'. A 'Continue' button with a green arrow icon is at the bottom left.

Field	Value	Unit
Bioconcentration Factor	175	
Concentration of concern	200	ug/L

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

- You are sent to the Exposure Factors Screen where you can review the defaults values. Any of these can be adjusted as necessary. Click on Continue button.

The screenshot shows the E-FAST software interface. The title bar reads 'E-Fast'. The menu bar includes 'Intro', 'General Pop Exp', 'Release Info', 'PChem', 'Exp Factors', and 'Fate'. The 'Exp Factors' menu item is selected. The main window is titled 'Exposure Factors' and contains a 'Help' button. Below the title, it says 'Chemical ID: Case A'. A list of exposure factors is displayed with their default values in input fields:

Body weight:	71.80	kg
Exposure duration (cancer):	30.00	years
Exposure duration (non cancer):	30.00	years
Averaging time (cancer):	75.00	years
Averaging time (non cancer):	30.00	years
Drinking water ingestion (chronic):	1.40	L/day
Drinking water ingestion (acute):	6.00	L/day
Fish ingestion (chronic):	6.00	g/day
Fish ingestion (acute):	129.00	g/day
Inhalation rate:	0.55	m3/hr

At the bottom left of the window is a 'Continue' button with a green arrow icon.

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

8. You are sent to the Fate Properties Screen where you will enter the percent removal in wastewater treatment (enter 50% for both high and low). Click on Calculate, Save Results, and Display Results button.

E-FAST

Intro | General Pop Exp | Release Info | PChem | Exp Factors | Fate

Fate Properties

Chemical ID: Case A

Waste water treatment removal (low): 50 %

Waste water treatment removal (high): 50 %

Drinking water treatment removal: 0.00 %

% removal via incineration: 0.00 %

% removal via fugitive: 0.00 %

Groundwater migration potential: Negligible

Calculate, save results, and display results pages

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

- Environmental Release Results are calculated and you get a message saying the file is saved to the A:\ drive. Click on OK. Click on River tab.

E-FAST

Intro | General Pop Exp | Release Info | PChem | Exp Factors | Fate | *Env. Rel. | *River | *PDM Site

Chemicals ID/Ref #
Case A.1

Environmental Release Results

Number of Sites: 1

	Water	Landfill/Sludge	Incineration	Fugitive
Total Releases: (before treatment)	6.00E+04 (kg/yr)	0.00 (kg/yr)	0.00 (kg/yr)	0.00 (kg/yr)
Release days/yr: (before treatment)	300.00			0.00
Per site release	200.00 (kg/site/day)	0.00 (kg/yr)	0.00 (kg/yr)	0.00 (kg/site/day)

Calculations Complete

Final report stored as a:\Case A.exp

OK

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

- Site-Specific Human and Aquatic Exposures to Surface Water Releases - Drinking Water Exposure Estimates Results are displayed. You can click on Fish Ingestion Information to view those exposure estimates.

E-FAST

Intro | General Pop Exp | Release Info | PCchem | Exp Factors | Fate | Env. Rel. | Rivers | PDM Site

Site-Specific Human And Aquatic Exposures to Surface Water Releases

Chemicals ID/Ref ID: Case A.1

Release Activity: Manufacture

Facility name: BOLLIVAR (N) WWTF

Facility location: BOLLIVAR NY 14715

NPDES: NY0022301

Reach Number: 05010001025

Reach Name: LITTLE GENESEE CR

Facility on reach? ☒ Yes ☐ No ☐ Unk.

Exposed Population: Adult

Discharge Type: Direct

WWT Removal: 50.00 %

Release days: 300.00

Pre-treatment release: 200.00 kg/day

Post-treatment release: 100.00 kg/day

Bio Concentration Factor: 175.00 L/kg

General Site Information | Drinking Water Information | Fish Ingestion Information

Drinking Water Exposure Estimates

Exposure Type	Results	ED (yr)	AT (yr)	IRW (kg)	IR (g/day)
Cancer					
LADDpot (mg/kg/day)	6.74E-03	30.00	75.00	71.00	1.40
LADDpot (mg/kg)	0.35	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADDpot (mg/kg/day)	1.69E-02	30.00	30.00	71.00	1.40
ADDpot (mg/kg)	0.06	30.00	30.00	NA	NA
Acute					
ADDpot (mg/kg/day)	0.17	1 day	1 day	71.00	6.00

E-FAST

Intro | General Pop Exp | Release Info | PCchem | Exp Factors | Fate | Env. Rel. | Rivers | PDM Site

Site-Specific Human And Aquatic Exposures to Surface Water Releases

Chemicals ID/Ref ID: Case A.1

Release Activity: Manufacture

Facility name: BOLLIVAR (N) WWTF

Facility location: BOLLIVAR NY 14715

NPDES: NY0022301

Reach Number: 05010001025

Reach Name: LITTLE GENESEE CR

Facility on reach? ☒ Yes ☐ No ☐ Unk.

Exposed Population: Adult

Discharge Type: Direct

WWT Removal: 50.00 %

Release days: 300.00

Pre-treatment release: 200.00 kg/day

Post-treatment release: 100.00 kg/day

Bio Concentration Factor: 175.00 L/kg

General Site Information | Drinking Water Information | Fish Ingestion Information

Fish Ingestion Exposure Estimates

Exposure Type	Results	ED (yr)	AT (yr)	IRW (kg)	IR (g/day)
Cancer					
LADDpot (mg/kg/day)	5.66E-03	30.00	75.00	71.00	6.00
LADDpot (mg/kg)	60.50	30.00	75.00	NA	NA
Chronic Non-Cancer					
ADDpot (mg/kg/day)	1.26E-02	30.00	30.00	71.00	6.00
ADDpot (mg/kg)	151.25	30.00	30.00	NA	NA
Acute					
ADDpot (mg/kg/day)	0.23	1 day	1 day	71.00	129.00

CASE STUDY A: Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

- Click on General Site Information to view Aquatic Exposure Estimates. Click on PDM Site tab to view PDM Site-Specific Aquatic Exposure estimates. Congratulations! You have your results. The CC will be exceeded **240 days per year**.

The screenshot shows the E-FAST General Population Exposure Module. The 'General Site Information' tab is selected. The 'Aquatic Exposure Estimates - Surface Waters' section is highlighted. The table below shows the results for the chemical release.

Flow description	Harmonic Mean	30q5	7q10	1q18
Flow (MLD)	95.10	49.94	30.54	25.29
Concentration (µg/L)	1891.57	2802.52	3274.93	3954.12

The screenshot shows the E-FAST PDM Site Specific Page. The 'PDM Site Specific Page' tab is selected. The 'PDM Site Specific Estimates' section is highlighted. The table below shows the results for the chemical release.

Flow description	Harmonic Mean	30q5	7q10	1q18
Flow (MLD)	95.10	49.94	30.54	25.29
Concentration (µg/L)	1891.57	2802.52	3274.93	3954.12

The 'PDM Site Specific Estimates' section shows the following results:

# Days exceeded:	238.52
% year exceeded:	65.62

Case Study B

Consumer Dermal Exposure

Uses the E-FAST
Consumer Exposure Pathway (CEM) Module

Case Study B: Consumer Exposure from Dermal Contact

Introduction

The purpose of this case study is to assess consumer exposure that may result from dermal contact with a proposed new additive to a consumer product. The Brown Manufacturing Corporation (BMC) is considering using Chemical C as a colorant in a new bar soap product. The BMC risk assessor must estimate potential consumer exposure to Chemical C before BMC product developers can make the decision to proceed with the new formulation. The assessor will use the E-FAST Consumer Exposure Module (CEM) to predict a Potential Lifetime Average Daily Dose (LADD) Rate, a Potential Average Daily Dose (ADD) Rate, and an Acute Potential Dose Rate (APDR) for a consumer from dermal contact with Chemical C in the soap product through hand and body washes.

The BMC risk assessor knows the following information about the proposed product and candidate Chemical C:

- Weight fraction of Chemical C in the final soap product will be 0.0025 - 0.0075 (percent by weight) (median = 0.005); and
- The chronic oral RfD for an adult (70 kg average body weight) for Chemical C is 0.02 mg/kg-day.

Estimation Of APDR, ADD and LADD Using CEM

Enter E-FAST (Figure C1). Proceed with the following steps:

1. Select Consumer Exposure Pathway Module (Figure C2);
2. Select Begin New CEM Run (Figure C2);
3. In the CEM Introduction Screen, enter Chemical Identification Information (Figure C3);
4. Click on the Scenario Tab (Figure C3);
5. Choose Bar Soap (Figure C4);
6. Click on Dermal Inputs Tab and view preset defaults (Figure C5). Any of these defaults can be overridden if necessary.
7. Click on Chemical Properties Tab and enter weight fraction information (Figure C6).
 - Median = 0.005
 - High end (90th%) = 0.0075;
8. Select Run the model (Figure C6).
9. Results are displayed. Click on Outputs-Dermal (Figure C6). Results can be saved in a WP file or printed.

Case Study B: Consumer Exposure from Dermal Contact

CEM Model Results

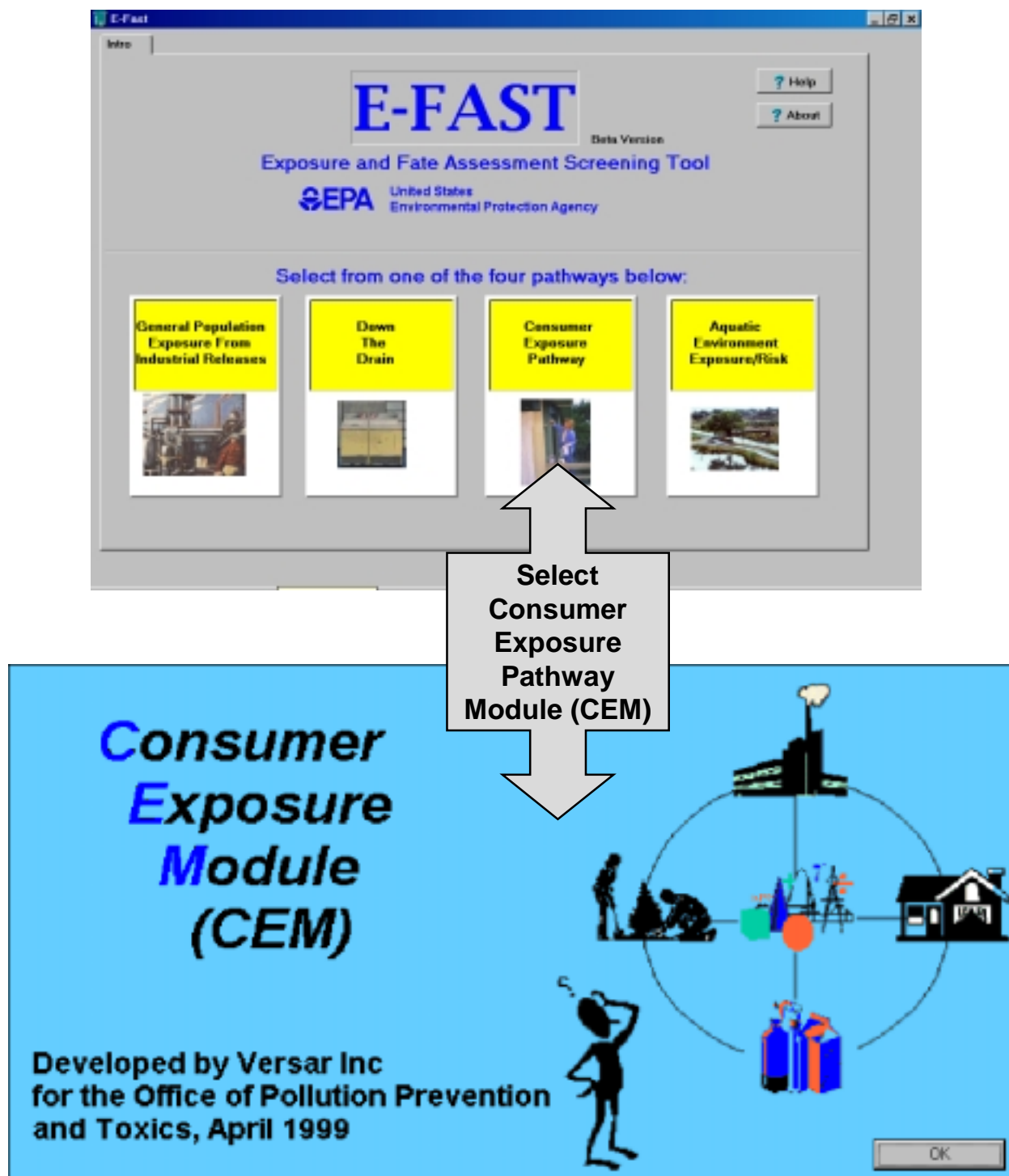
After running the CEM model, the BMC risk assessor obtained the following predicted exposure results (see Figure C6):

LADD	=	2.71e-03 mg/kg-day
ADD	=	2.75e-03 mg/kg-day
APDR	=	4.52e-03 mg/kg-day

In-house studies have demonstrated that the **dermal absorption fraction** of Chemical C is 10 to 20 percent of the applied dose. Using the more conservative value of 20 percent absorption, the assessor will adjust the predicted ADPR 4.52e-03 mg/kg-day to obtain a predicted absorbed adult dose of 8.984e-04 mg/kg-day. This is below the reported adult chronic oral RfD for Chemical C of 2.00e-02 mg/kg-day. The assessor will report to product developers that the amount of Chemical C in the soap formulation will not exceed the chronic oral RfD for Chemical C.

Case Study B: Consumer Exposure from Dermal Contact

Figure C1
E-FAST Opening Screen



Case Study B: Consumer Exposure from Dermal Contact

Figure C2
CEM Opening Screen

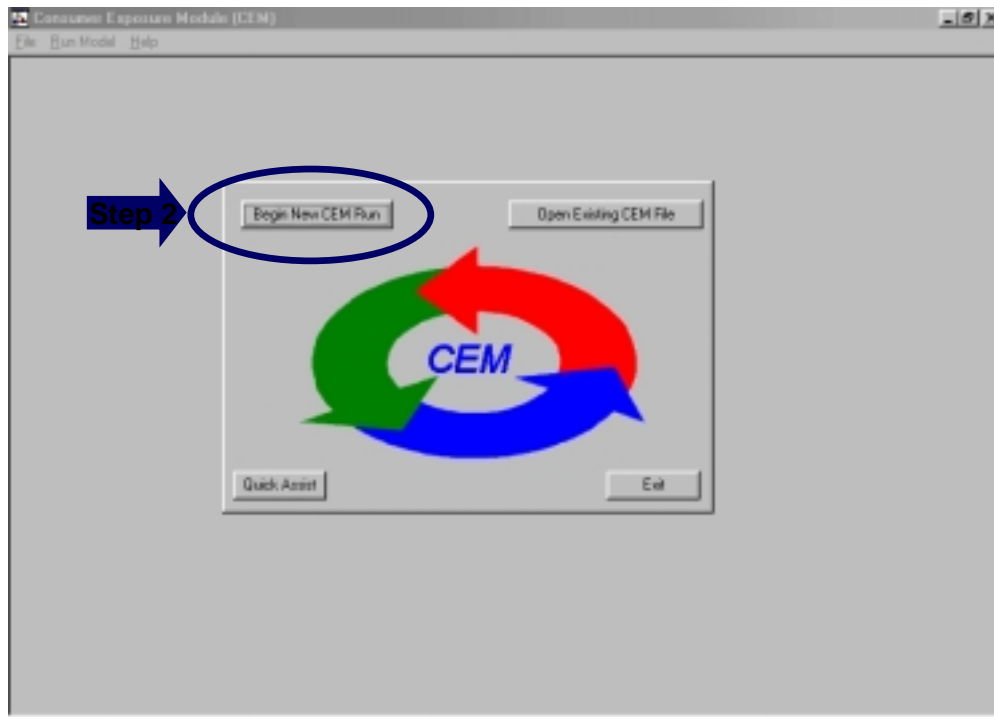
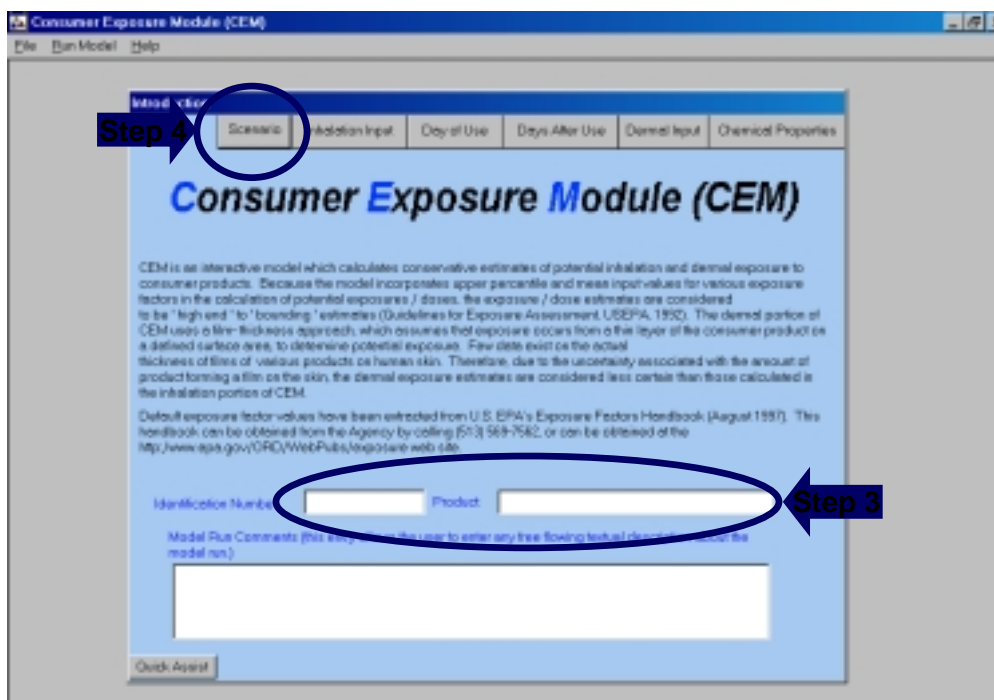


Figure C3
CEM Introduction Screen



Case Study B: Consumer Exposure from Dermal Contact

Figure C4
Dermal Scenario Selection Screen

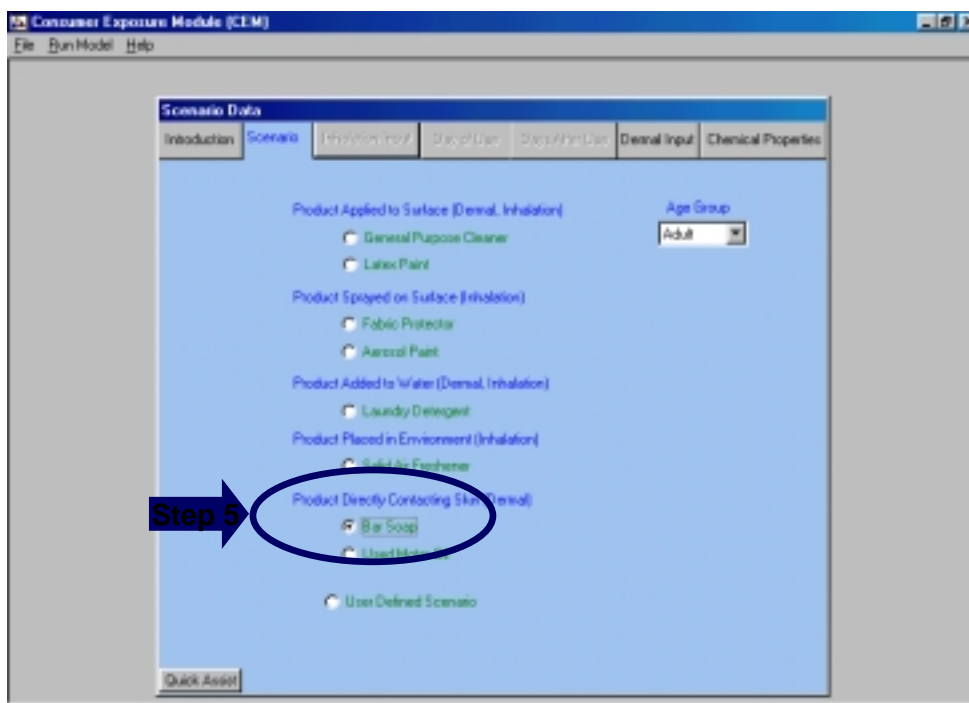
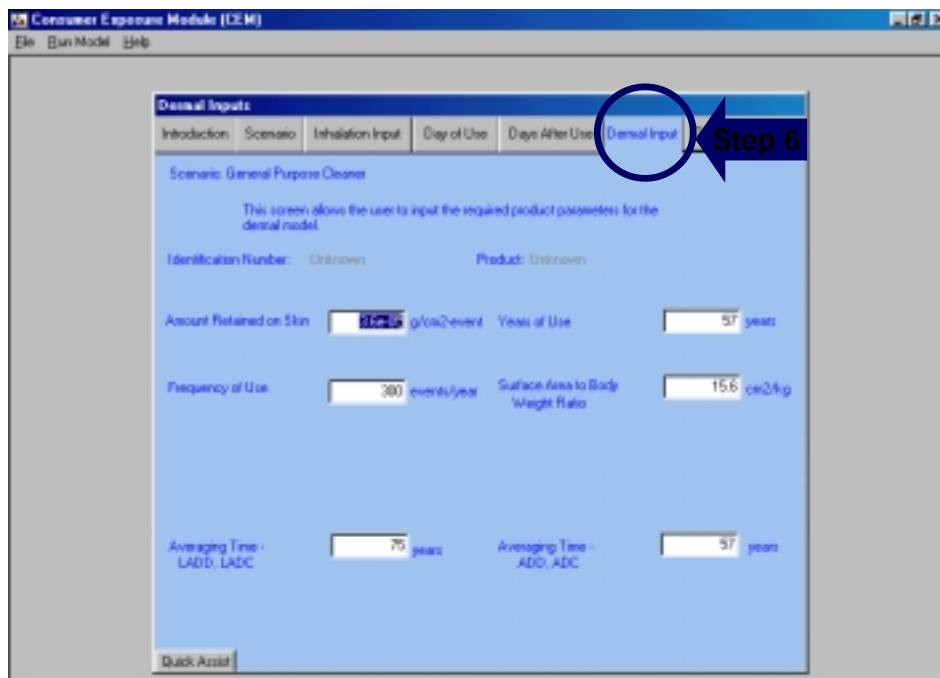


Figure C5
Dermal Scenario Input Screen



Case Study B: Consumer Exposure from Dermal Contact

Figure C6
CEM Model Inputs

Chemical Properties

Introduction Scenario **Input/Output** Day of Use Days After Use Dermal Input Chemical Properties

Scenario: Bar Soap

This screen allows the user to input the required physical and chemical properties of the product required for the models.

Identification Number: Unknown Product: Unknown

Chemical Name:

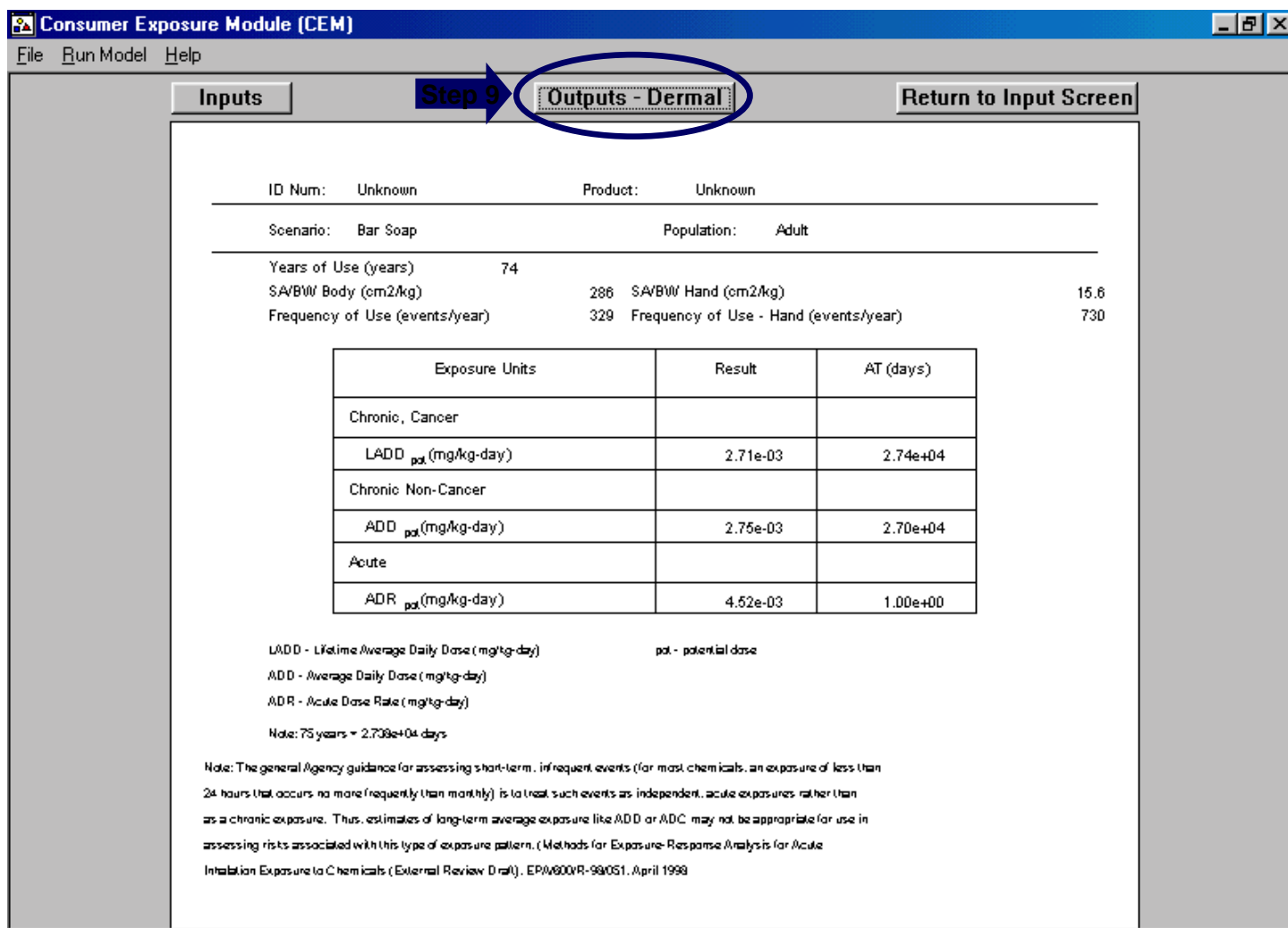
Weight Fraction - Median: unitless

Weight Fraction - 90th %: unitless

Quick Assist

Case Study B: Consumer Exposure from Dermal Contact

Figure C6
CEM Model Results



Case Study C

Workplace Release and Exposure

Uses the Chemical Screening Tool for Exposures and Environmental Releases

(ChemSTEER)

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures Inputs for the Scenario

Mock PMN Information

Since one of the primary uses of ChemSTEER by EPA is for assessing new chemicals submitted for PMN review under TSCA Section 5, we have created a mock set of input values that are consistent with information typically submitted for a new chemical review.

Brief Description of the Scenario

The chemical that is being assessed is a semivolatile liquid used as a chemical intermediate. It is manufactured in formulation at a concentration of 80%. The formulation is then sold to other facilities to be used in other reactions (i.e., the chemical will be destroyed in the reactions).

The manufacturers perform QC sampling of the formulation before it is loaded into drums for distribution to the users. The manufacturers also clean the reactor vessel once every 5 batches.

The users receiving the drums of the intermediate formulation containing the chemical (at a concentration of 80%), pump it from the drums and into the process. When a drum is emptied, the residues are rinsed with a solvent that is subsequently incinerated.

Information About the Chemical to be Assessed

- ❖ Production volume (PV) = 100,000 kg/yr
- ❖ Name = "Case Study Chemical"
- ❖ Molecular weight = 150
- ❖ Vapor pressure = 1 torr
- ❖ Density = 0.815 g/cm³

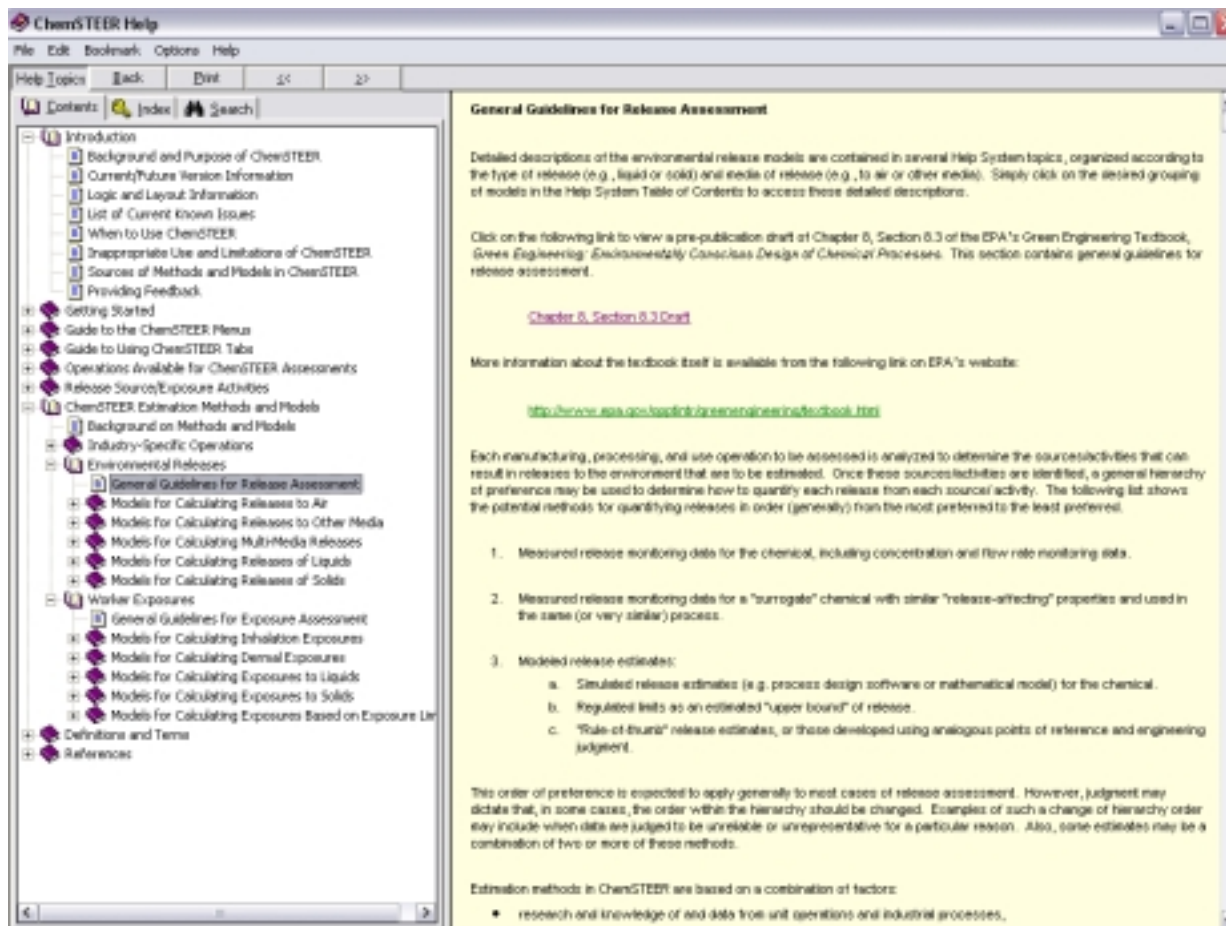
Information About the Manufacture

- ❖ Performed at one site
 - ❖ Batch size is 1,000 kg of the formulated product (80% chemical) per batch
 - ❖ 12 hours per batch; 1 batch per day
 - ❖ Process description:
 Reactants are added to reactor -> Formulation (80% chemical) sampled -> Formulation loaded into 40-gallon drums for distribution to user sites -> Reactor vessel is rinsed with water every 5 batches
 - ❖ 4 workers performing sampling, drumming, and reactor cleaning activities:
- | Activity | Concentration | # Workers | Hrs/day | Days/yr |
|------------------|---------------|-----------|-------------------------------------|---------|
| Sampling | 80% | 4 | 0.02 | 125 |
| Drumming | 80% | 4 | ChemSTEER will estimate hpd and dpy | |
| Cleaning reactor | < 80% | 4 | 1.5 | 25 |

Information About the Use

- ❖ Use rate = 10 kg formulation per site, per day (formulation contains 80% chemical)
 - ❖ Use sites operate 250 days per year
 - ❖ Process description:
 Formulation containing 80% chemical is metered from drum into the process -> chemical is destroyed in the reaction/converted to a new substance -> empty drums are rinsed with solvent before disposal -> used solvent is incinerated
 - ❖ 3 workers per site are involved in handling the formulation containing the chemical:
- | Activity | Concentration | # Workers | Hrs/day | Days/yr |
|-------------|---------------|-----------|-------------------------------------|-----------------------------|
| Unloading | 80% | 3 | ChemSTEER will estimate hpd and dpy | |
| Drum rinses | <80% | 3 | 0.5 | ChemSTEER will estimate dpy |

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures Help System



The ChemSTEER Help System

The ChemSTEER Help System has been developed in order to provide you with extensive descriptions of how ChemSTEER is organized, as well as how the release and worker exposure estimates are made in an assessment. This includes full documentation on each of the methods and models that are used to perform the calculations (e.g., input parameters, default settings and values, equations used, and associated logic algorithms).

All users are strongly encouraged to review this Help System prior to creating their first assessment and to utilize it regularly as a resource to assist in future assessments. Taking the time to learn and understand the complex functions of this tool will enable you to perform screening-level assessments of environmental releases and worker exposures with greater ease and flexibility.

To access the ChemSTEER Help System, click on the **Help** menu item and select **Index**. Then, simply select a topic from the menu on the left and view the content in the screen on the right.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The General Tab

ChemSTEER 10/31/2002 Version - Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

General

Assessment Type: PMN Date: 1/13/2003 CBI: No

Status: Pre-review draft Revision: ENG Assessor comments: No

Identifier: Case Study - Mock PMN Number of Contact Reports: 0

Assessor:

Name: Scott Prothero L. Crawford

Affiliation: U.S. EPA ERG, Inc. (contractor)

Phone: 202-555-1234 404-555-0987

Email: prothero.scott@epa.gov leslie.crawford@erg.com

Company Name: XYZ Chemical Co. Contact Information:

Street Address: 1313 Mockingbird Lane Mr. O.B. Kenobi

City: Anywhere (999) 555-3456

State: AK Zip: 99999

Update General Information View/Update Contact Report(s) View/Update Comments

Entering General Information About the Assessment

When you click the **General** tab, a screen displaying general information about the assessment is shown.

To add or modify the General information, click the **Update General Information** button.

1. Select the Assessment Type – choose from this list of various EPA labels to describe assessment types that EPA uses ChemSTEER to perform.
2. Enter an assessment Identifier – Enter a descriptive unique title in this field. This field will be the saved “name” of your assessment and is the primary means of identifying this assessment among a list of assessments in a single ChemSTEER database file.
3. Verify/modify the Date of the assessment – this field is automatically populated with the current date for a new assessment. You should enter a new date to reflect when the assessment was completed.
4. Enter Assessor information: you may enter the name, affiliation, phone number, and email address for one or two assessors (i.e., persons preparing the assessment).
5. Enter the Company information: you may enter the company name, address, city, state, zip code, and contact information for the assessment.

Note: Status and Revision options are used for internal EPA reports and may be left incomplete.

When you click the **View/ Update Comments** tab, a screen displaying a text field is shown. You may enter key information about the assessment here.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Chemical* Tab

ChemSTEER 10/31/2002 Version - Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Chemical

Chemical Name: Case Study Chemical

Chemical Category:

Trade Name(s):

Chemical CAS Number: 999-99-9 Molecular Formula:

Total Assessed Production Volume (PV): 100000 kg/yr Type of Notice: Manufacturing

Imported Production Volume (PVi): kg/yr

Domestic Production Volume (PVd): 100000 kg/yr

Vapor Pressure (VPchem): 1 torr at 20 C

Molecular Weight (MW): 150 g/mol % < 500: % < 1000:

Density (Dchem): 0.815 g/cm3 at C

Solubility in Water (Wschem): g/L at C

General Description of End Use(s): Chemical intermediate for off-site reactions

View/Update Exposure Limits Update Chemical Information View/Update Regulatory Limits

Parameters with red labeling are often important defaults used in mass balance, container, and model calculations.

Entering Information About the Chemical to be Assessed

When you click the **Chemical** tab, a screen displaying information about the chemical being assessed is shown.

To add or modify information about the chemical, click the **Update Chemical Information** button.

Enter the following information about the chemical being assessed in the appropriate fields:

- *Chemical name*
- *Chemical category*
- *Trade name(s)*
- *CAS number (if known)*
- *Molecular formula*
- *Domestic production volume* (PVd, kg/yr) – the annual amount of the chemical to be assessed that is manufactured domestically
- *Imported production volume* (PVi, kg/yr) – the annual amount of the chemical to be assessed that is imported to the U.S.
- *Total assessed production volume* (PV, kg/yr) – the total annual amount of the chemical to be assessed (PV = PVd + PVi); ChemSTEER automatically sums your entries for PVd and PVi, and displays PV

**Note: PV is the most often used parameter throughout most assessments. VP, MW, Dchem, and Wschem may be needed depending upon which release or exposure models are used in the assessment.*

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Chemical* Tab (continued)

ChemSTEER 10/31/2002 Version - Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Chemical

Chemical Name: Case Study Chemical

Chemical Category:

Trade Name(s):

Chemical CAS Number: 999-99-9 Molecular Formula:

Total Assessed Production Volume (PV): 100000 kg/yr Type of Notice: Manufacturing

Imported Production Volume (IPV): kg/yr

Domestic Production Volume (IPVd): 100000 kg/yr

Vapor Pressure (VPchem): 1 torr at 20 C

Molecular Weight (MW): 150 g/mol % < 500: % < 1000:

Density (Dchem): 0.815 g/cm3 at C

Solubility in Water (WSchem): g/L at C

General Description of End Use(s): Chemical intermediate for off-site reactions

View/Update Exposure Limits Update Chemical Information View/Update Regulatory Limits

Parameters with red labeling are often important defaults used in mass balance, container, and model calculations.

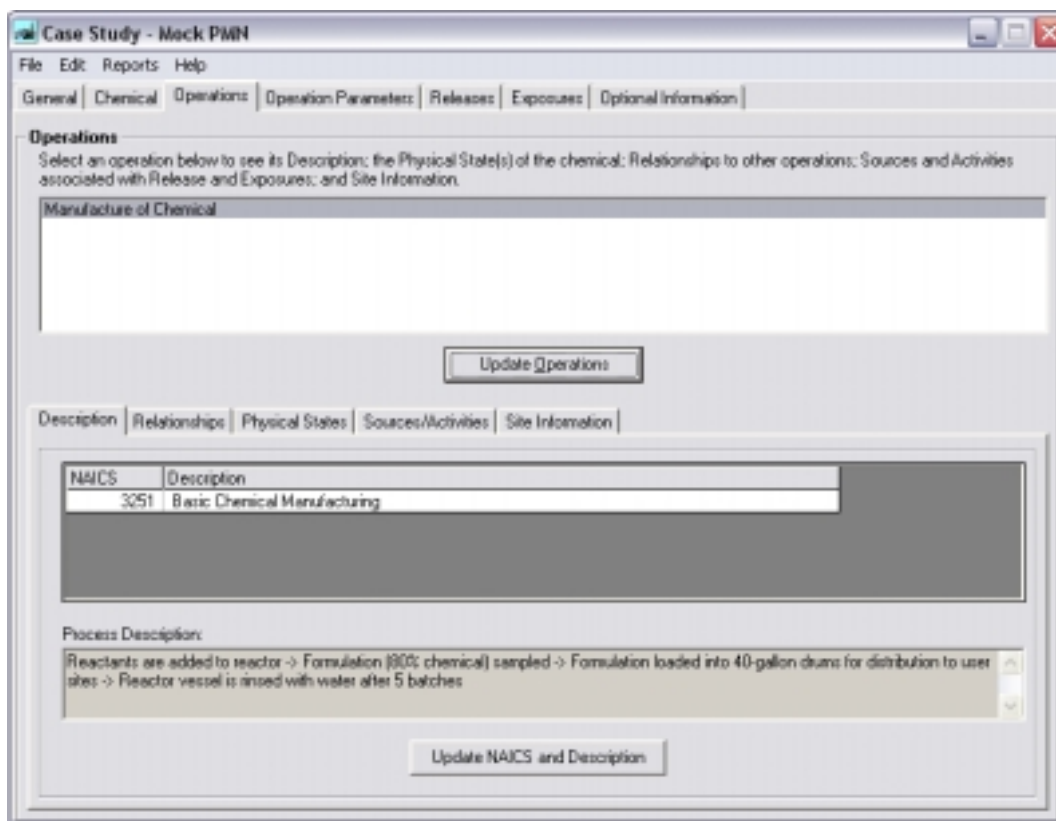
Entering Information About the Chemical to be Assessed (continued)

Enter the following information about the chemical being assessed in the appropriate fields:

- **Vapor pressure** (VPchem, torr) – the vapor pressure of the pure chemical to be assessed; you may also enter the reference temperature (°C) for this value
- **Molecular weight** (MW, g/mol) – the molecular weight of the chemical to be assessed
- % < 500 g/mol and % < 1000 g/mol – for use with high molecular weight polymers; indication of the distribution of molecular weight of the chemical to be assessed.
- **Density** (Dchem, g/cm³) – the density of the pure chemical to be assessed; you may also enter the reference temperature (°C) for this value
- **Solubility in water** (WSchem, g/L) – the solubility of the pure chemical in water; you may also enter the reference temperature (°C) for this value or simply check the box indicating the chemical is 'dispersible'
- **General description of end use(s)**

**Note: PV is the most often used parameter throughout most assessments. VP, MW, Dchem, and Wschem may be needed depending upon which release or exposure models are used in the assessment.*

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The Operations Tab



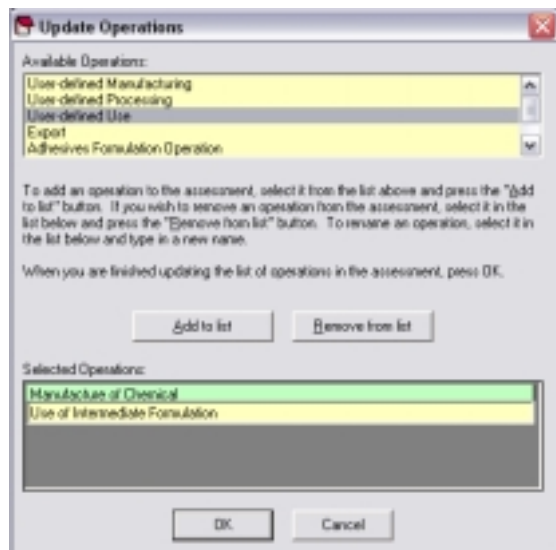
The Operations Tab

Click on the **Operations** tab and each of its subtabs to build your scenario and enter necessary information about each operation in your assessment.

Choosing Operations for the Scenario

The first step in building a scenario to be assessed is to choose the operations.

Begin by clicking the **Update Operations** button to choose the operations in your scenario.



At the top of the **Update Operations** screen is a list of *Available Operations* that you may choose.

To select an operation, you may either double-click on it or click it once and then click the **Add to list** button.

The selected operation then appears in the *Selected Operations* list at the bottom of the **Update Operations** screen. Continue this process for each operation you wish to include in your assessment.

Renaming Operations

It is helpful to rename the operations to better describe your assessment. To do this, select the operation by clicking on it in the *Selected Operations* list and enter the new name (e.g., *Manufacture of Chemical*).

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operations* Tab (continued)

Case Study - Mack PMN

File Edit Reports Help

General Chemical **Operations** Operation Parameters Releases Exposures Optional Information

Operations

Select an operation below to see its Description; the Physical State(s) of the chemical; Relationships to other operations; Sources and Activities associated with Release and Exposures; and Site Information.

Manufacture of Chemical

Update Operations

Description Relationships Physical States Sources/Activities Site Information

NAICS	Description
3251	Basic Chemical Manufacturing

Process Description:

Reactants are added to reactor -> Formulation (80% chemical) sampled -> Formulation loaded into 40-gallon drums for distribution to user sites -> Reactor vessel is rinsed with water after 5 batches

Update NAICS and Description

Entering Operation Descriptions

You may enter North American Industrial Classification System (NAICS) codes and other descriptions associated with each operation of the assessment by clicking on the **Description** subtab within the **Operations** screen.

Select the desired operation at the top of the **Operations** screen and click the **Update NAICS and Description** button to view the **Update Operation Description** screen.

1. To add an associated NAICS code, click the **Add/Remove NAICS** button and select a NAICS code from the list of codes.
2. You may also enter further details about the selected operation by typing them within the *Process Description* box in the **Update Operation Description** screen.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operations* Tab (continued)

Case Study - Mock PMN

File Edit Reports Help

General Chemical **Operations** Operation Parameters Releases Exposures Optional Information

Operations

Select an operation below to see its Description; the Physical State(s) of the chemical; Relationships to other operations; Sources and Activities associated with Release and Exposures; and Site Information.

Manufacture of Chemical
Use of Intermediate Formulation

Update Operations

Description **Relationships** Physical States Sources/Activities Site Information

Subsequent Operations: **PVop: 100,000** **PVI: 100.00 %**

Subsequent Operation	Fraction of PV	PVop (kg/yr)
Use of Intermediate Formulation	100	100000

Update Relationships

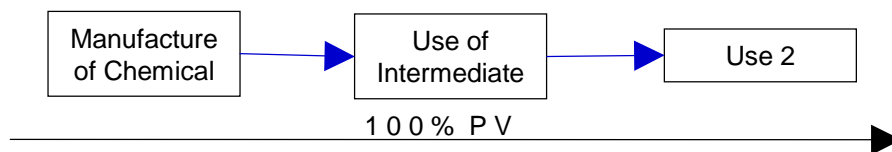
Select the operations in the list at the top of this page in order from first to last to allow ChemSTEER to automatically distribute the assessed volume properly (e.g., manufacturing first, then processing1, processing2, ..., use1, use2, ...).

Defining Operation Relationships

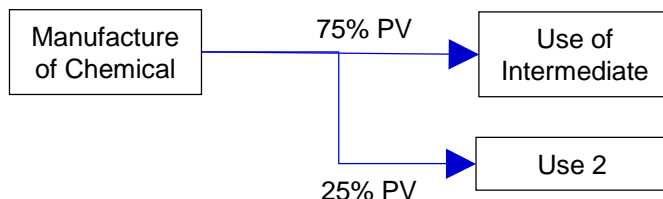
The next step in building your assessment scenario is to indicate the relationships of your chosen operations (i.e., the order in which they are performed). Click on the **Relationships** subtab in the **Operations** screen.

Select the desired operation at the top of the **Operations** screen to view the current settings: subsequent operation(s), fraction of PV, and PV in each subsequent operation. Click the **Update Relationships** button to modify any of these relationship settings.

For example, if we had chosen a second use operation for the manufactured chemical formulation, ChemSTEER defaults to a simple, straight series relationship:



The **Relationships** subtab can be used to modify the relationship to:



Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operations* Tab (continued)

ChemSTEER 10/31/2002 Version - Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Operations

Select an operation below to see its Description; the Physical State(s) of the chemical; Relationships to other operations; Sources and Activities associated with Release and Exposures; and Site Information.

Manufacture of Chemical
Use of Intermediate Formulation

Update Operations

Description Relationships Physical States Sources/Activities Site Information

	Physical State	Other Information
Chemical into the Operation:		NA - chemical is manufactured
Chemical out of the Operation:	Formulation	100% chemical in reaction mixture
Chemical in the Operation:		

Update Physical State

Defining Physical State(s) of the Chemical

You should enter information pertaining to the physical state of the chemical being assessed within each operation by clicking on the **Physical States** subtab within the **Operations** screen.

Appropriate terms would include liquid, solid, vapor, gas with additional modifiers if needed (e.g., molten liquid, etc.). Formulation (as shown above) should not be used as it does not adequately describe physical state.

Select the desired operation at the top of the **Operations** screen and click the **Update Physical State** button.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operations* Tab (continued)

Case Study - Mack PMN

File Edit Reports Help

General Chemical **Operations** Operation Parameters Releases Exposures Optional Information

Operations

Select an operation below to see its Description; the Physical State(s) of the chemical; Relationships to other operations; Sources and Activities associated with Release and Exposures; and Site Information.

Manufacture of Chemical
Use of Intermediate Formulation

Update Operations

Description Relationships Physical States **Sources/Activities** Site Information

Sources and Activities associated with releases and exposures within the operation:

Activity	Release	Exposure
Sampling Liquid Product	Yes	Yes
Loading Liquid Product into Drums	Yes	Yes
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	Yes	No

Update Sources/Activities

Identifying Operation Sources/Activities

For each operation of the assessment, you must identify at least one release source or worker activity for which ChemSTEER will calculate estimated releases and/or exposures by clicking on the **Sources/Activities** subtab within the **Operations** screen.

This selection is critical, as it will determine which default release/exposure models are used for the calculations.

Select the desired operation at the top of the **Operations** screen and click the **Update Sources/Activities** button.

Sources/Activities are listed under categories shown in the *available sources/activities* list. To view or hide the list of specific sources/activities, double-click on the category of interest.

Select the source/activity by either double-clicking on it or clicking it once and then clicking the **Add to list** button.

Update Operation Sources/Activities

Selected Operation: **Manufacture of Chemical**

Double-click on the category of interest in the following list to view/hide available sources/activities:

- Cleaning Liquid Residuals from Transport Containers/Vessels
- Cleaning Solid Residuals from Transport Containers/Vessels
- Coating Applications
- Equipment Cleaning Losses of Liquids
 - Equipment Cleaning Losses of Liquids from a Single, Large Vessel**
 - Equipment Cleaning Losses of Liquids from a Single, Small Vessel
 - Equipment Cleaning Losses of Liquids from Multiple Vessels

Select sources/activities from the list above in order to include them in the current operation. You can rename a selected source/activity by clicking on it in the list below and typing in a new name. Be sure to set the Release column to "Yes" if the exposure model requires a vapor generation rate (G). (See Help for more detail)

When you are finished updating the sources/activities in the operation, press OK.

Add to list Remove from list

Sources/Activities that will be accessed in the operation:

Activity	Release	Exposure
Sampling Liquid Product	Yes	Yes
Loading Liquid Product into Drums	Yes	Yes
Equipment Cleaning Losses of Liquids from a Single, Large Vessel	Yes	No

OK Cancel

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operations* Tab (continued)

Case Study - Mock PMN

File Edit Reports Help

General Chemical **Operations** Operation Parameters Releases Exposures Optional Information

Operations

Select an operation below to see its Description; the Physical State(s) of the chemical; Relationships to other operations; Sources and Activities associated with Release and Exposures; and Site Information.

Manufacture of Chemical
Use of Intermediate Formulation

Update Operations

Description Relationships Physical States Sources/Activities **Site Information**

Operation Site Information:

Facility Name	Address	City	State	Zip	County
XYZ Chemical Co.	1313 Mockingbird Lane	Anywhere	AK	99999	

Update Site Information

Entering Operation Facility Information

You may enter information regarding the facility or facilities that are performing the operations of the assessment by clicking the **Site Information** subtab within the **Operations** screen.

Select the desired operation at the top of the **Operations** screen and click the **Site Information** button.

If you have no information about the facility or facilities for the operation, type “unknown” in the Facility Name field.

NOTE: Sufficient information about the facility location(s) will usually prevent the use of the most conservative assumptions (e.g., lowest stream flow) for the environmental exposure portion of the EPA exposure assessment.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The Operation Parameters Tab

Parameter	Type	Value
BMInchem: Batch Mass Input of Chemical	Default/Derived	0
BMOutchem: Batch Mass Output of Chemical	Default/Derived	800
BMInrm: Batch Mass Input of Raw Material	Default/Derived	0
BMOutprod: Batch Mass Output of Product	User Specified	1,000
NS: Number of Sites	User Specified	1
Nbyr: Number of Batches per Year	Default/Derived	125
Yrm: Weight Fraction of Chemical in Raw Material	Default/Derived	0
Yprod: Weight Fraction of Chemical in Product	User Specified	0.8
HB: Hours per batch	User Specified	12
ODmax: Maximum number of operating days	User Specified	365
Nbld: Number of batches per line per day	Default/Derived	1.0
Ls: Lines per site	Default/Derived	1
OD: Number of Operating Days	Default/Derived	125
Nbld: Number of Batches per Day	Default/Derived	1

The Operation Parameters Tab

Click on the **Operation Parameters** tab and each of the subtabs to verify or edit the default values for key operation parameters (e.g., mass balance of chemical into and out of the operation, calculation of the number of containers filled and/or emptied during the operation).

Entering Mass Balance Parameters

ChemSTEER allows a great amount of flexibility in which input parameters can be entered for each assessment.

We will set the mass balance parameters for the *Manufacture of Chemical* operation:

1. Click the **Update Parameters** button to enter the mass balance parameters for the selected operation.
2. **Mass Accounting Basis Selection - Continuous or Batch processes:** Continuous processes run 24 hours per day over a number of days per year; Batch processes occur over less than 24 hours, thus an operation may perform one or more batches per day.
3. **Mass Accounting Basis Selection - Influent or Effluent basis:** Influent basis causes ChemSTEER to utilize the current settings for the chemical as it enters the selected operation (e.g., utilizing the settings for the chemical exiting the previous operation in a series). Effluent basis causes ChemSTEER to utilize the current settings for the chemical as it exits the selected operation.

❖ For the *Manufacture of Chemical* operation, we will select a *Batch* process with an *Effluent* basis.

Strategy: If you know more about the product of an operation (i.e., typical production rates and composition of the chemical within the product), selecting *Effluent* as the basis is often the most practical strategy. Similarly, if more is known about the use of the chemical as a raw material for the selected operation, selecting *Influent* is often the best approach.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures

The Operation Parameters Tab (continued)

Update Operation Mass Accounting Parameters

Manufacture of Chemical

Mass Accounting Basis Selection: **Specify Mass Balance Input Parameters** | Specify Other Batch Parameters

Please specify exactly three of the first five parameters, including at least one parameter from the first 'pair' and at least one parameter from the second 'pair.' ChemSTEER will calculate the other two parameters for you. If you only need a smaller subset of these parameters for use in a linked set of models, enter only those parameters and ChemSTEER will not derive a complete set of default values.

Batch Operation: Using Effluent

Parameter	Value	Action
<input checked="" type="checkbox"/> NS: Number of Sites	1	Calculate
<input type="checkbox"/> Nby: Total batches per year	125	Defaults
<input checked="" type="checkbox"/> Yprod: Weight Fraction of Chemical in Product (unitless)	0.8	Calculate
<input checked="" type="checkbox"/> BMOprod: Batch Mass Output of Product kg/site-batch	1000	Calculate
<input type="checkbox"/> BMOchem: Batch Mass Output of Chemical kg/site-batch	800	Calculate

Buttons: Calculate remaining two parameters | Restore Defaults

Batch Influent Parameters Calculation

If appropriate, you may change one or two of the following three parameters and press the 'Recalc' button for the parameter you wish to have ChemSTEER recalculate. Once you have changed one of these parameters, you must press a 'Recalc' button before you close this window.

Parameter	Value	Action
<input type="checkbox"/> Yrm: Weight Fraction of Chemical in Raw Material (unitless)	0	Recalc
<input type="checkbox"/> BMrm: Batch Mass Input of Raw Material kg/site-batch	0	Recalc
<input type="checkbox"/> BMchem: Batch Mass Input of Chemical kg/site-batch	0	Recalc

Buttons: Calculate defaults

Buttons: OK | Cancel | Back | Help

Entering Mass Balance Parameters (continued)

4. *Specify Mass Balance Input Parameters* - The second subtab contains the input parameters that ChemSTEER utilizes to calculate the remaining mass balance parameters. You must specify exactly three of the five parameters listed in upper portion of this subtab.

5. For the *Manufacture of Chemical* operation, it is known that the manufacturers: a) operate one site (NS); b) that the product formulation contains 0.8 kg chemical/kg formulation (Yprod) (i.e., 80% chemical; and c) that 1,000 kg of formulation is produced in each batch (BMOprod).

6. When you have completed entering the three known parameters, click on the **Calculate remaining two parameters** button.

❖ After entering the three known values, ChemSTEER determines that the site must perform 125 batches per year (Nby) in order to process the amount of chemical being assessed (PV = 100,000 kg/yr) and that 800 kg of chemical is manufactured in each batch (BMOchem).

Since the chemical is created in this operation, the input parameters listed in the lower half of the screen are not applicable in this case.

In addition, by clicking the **Specify Other Batch Parameters** subtab additional parameters may be specified (e.g., hours per batch).

***Note:** You are highly encouraged to review this topic in the **ChemSTEER Help System** for a more complete description (refer to *Guide to Using ChemSTEER Tabs – Operation Parameters Tab – Mass Balance Parameters Subtab*).

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Operation Parameters* Tab (continued)

Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Operation Parameters

Manufacture of Chemical
Use of Intermediate Formulation

Mass Balance Parameters: Container Parameters

Sources/Activities that are associated with containers are shown in two of the four tabs below. Double click on any row to update it.

For Raw Material For Product For Other Material Container Parameters by Activity

OD = 125

Source/Activity Name	Ncy (containers / site-year)	ODa (days/yr)	Ncd (containers / site-day)	t (containers / hour)	QHa (hours / day)
Loading Liquid Product into Drums	1013.04	125	8.1043	20	0.4052

Entering Container Parameters

The **Container Parameters** subtab allows you to verify and/or edit the default settings for how the mass balance around loading and unloading containers with materials containing the chemical.

We will set the container parameters for the *Manufacture of Chemical* operation.

The **Container Parameters** subtab displays the list of container-related sources/activities that were chosen for the selected operation (e.g., loading liquid product into drums) along with the current values for the key container parameters (for new assessments these are ChemSTEER default values).

Container Parameters

Verify/Select Container Parameters for Product Verify/Select Container Parameters by Source/Activity

Loading Liquid Product into Drums

Verify or change the container information below. (To press OK, to return to the main window. Please note that you may update Yc and Dc in order to derive MCD, or you may uncheck Yc and Dc and enter MCD yourself.)

Yprod: Weight fraction of chemical in product (unitless) 0.8

Sprod: S (kg/containers) 1

Dprod: Density of product (kg/L) 0.875

Fc: Fraction of total volume shipped in this container (unitless) 1

☒ Derive MCD

Vc: Volume Capacity of container (gal) 40

Dc: Density of (kg/L) 0.875

☐ Specify MCD directly

MCD: Mass Capacity of container (kg/containers) 1320.000

Yc: Weight fraction of chemical (unitless) 0.0

OK Edit Restore Defaults Cancel

These sources/activities can be viewed according to what type of material is handled by clicking on each of the subtabs, **Raw Material**, **Product**, or **Other Material**. Additional parameters are summarized in the **Container Parameters By Activity** subtab.

1. **Verify/Select Container Parameters** - Double-click on a container-related source/activity to view the **Verify/Select Container Parameters for Product** subtab.

As a default, ChemSTEER assumes the volume of each drum (Vc) is 55 gallons. By changing Vc from 55 to 40 gallons, the number of drums filled per year is adjusted using this new volume, as well as the chemical density and total PV.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures

The *Operation Parameters* Tab (continued)

Entering Container Parameters (continued)

2. *Verify/Select Container Parameters* – Click the ***Verify/Select Container Parameters by Source/Activity*** subtab.

❖ Approximately 1,013 drums of our chemical formulation will be filled over the 125-batch campaign and approximately 8 drums will be filled per day.

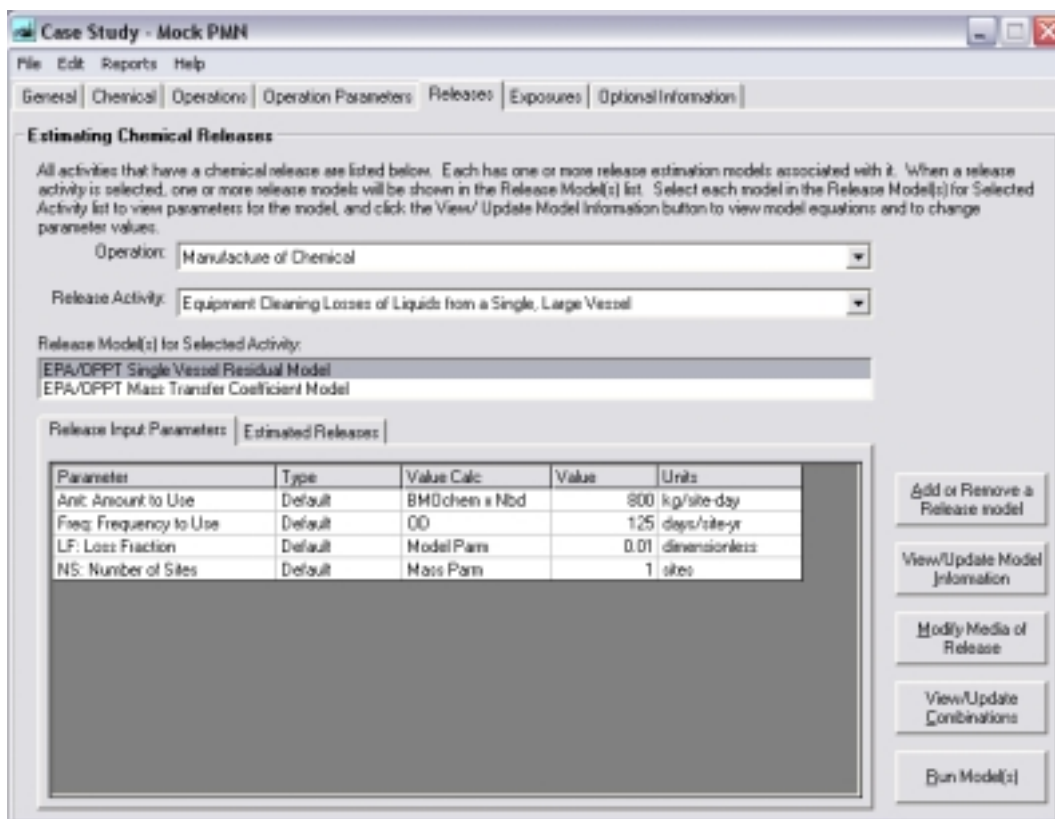
❖ The default drum unloading rate is 20 drums per hour, which determines the total number of hours (OHa) spent filling the drums each day.

3. You may choose three parameters in this screen to specify and ChemSTEER will adjust the remaining two parameters accordingly. Let's assume that in our scenario, the loading rate is 4 drums per hour. We will specify: a) the total days per year (ODa) is kept at 125 days/year; b) the number of drums filled per day (Ncd) is kept at 8.1043 drums/site-day; and 3) the drum fill rate (r) is changed from 20 to 4 drums/hr.

❖ After clicking the ***Calculate remaining two parameters*** button, ChemSTEER determines that: the number of containers filled per year (Ncy) is approximately 1,013 drums/year; and it will take slightly longer than 2 hours/day to fill them (OHa). OHa is used later to calculate fugitive releases and inhalation exposures.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures

The Releases Tab



The Releases Tab

Click on the **Releases** tab to view or modify the models (i.e., algorithms) and associated input parameters used to calculate the releases to water, air, incineration, and/or landfill from each of the chosen sources within each of the operations of your assessment. Then click Run Model(s) to generate release estimate results from the model(s).

1. Select an operation from the *Operation* drop down list.
2. Select a source for which releases are calculated from the *Release Activity* drop down list.

❖ The models that are used to calculate the releases from the selected source within the selected operation appear in the *Release Model(s) for Selected Activity* box.

❖ The parameters used by the selected release model appear in the **Release Input Parameters** subtab. This subtab also indicates which parameters are ChemSTEER default values, the source of the parameter value (i.e., whether previously input in another tab or calculated from other input parameters), the current value, and the units.

***Note:** ChemSTEER currently contains over a dozen different models that can be used to calculate releases, each with their own set of default settings and values. You are highly encouraged to review the *ChemSTEER Estimation Methods and Models – Environmental Releases* in the **ChemSTEER Help System** for a more complete description of the models and their bases before selecting alternative models to the ChemSTEER defaults and/or modifying default input values.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Releases* Tab (continued)

Adding or Removing Release Models

Click on the **Add or Remove a Release Model** button in the **Releases** screen to change the default models that are used for the selected release source.

The **Add/Remove Release Models** screen will appear with a list of the most appropriate alternative models for the selected release source.

Read-only and updatable information about the selected release model, including the model equation, mechanism, basis, and input parameters are listed below. Because the release can be calculated using several valid equations for this model, all of the possible parameters that may be used are listed in the Input Parameters grid. Depending on the data values for this release, some of these parameters will not be required. To view options or change a parameter value, click on the label for that parameter under the Type column. When Type is User-defined, you must click on the cell under the value column and type in your own value.

Activity: Equipment Cleaning Losses of Liquids from a Single, Large Vessel
Model: EPA/OPPT Single Vessel Residual Model

Model Equation: $DIR \text{ (kg/site-day)} = LF \times Amt$
 $DIR \text{ occurs over [Freq] days/year}$

Mechanism: Residual removed from and/or disposed from a single process vessel

Basis: EPA/OPPT Single Vessel Residual Model, CEB standard 1% residual.

Parameter	Type	Value Calc	Value	Units
Amt: Amount to Use	Default	BMIOchem x Nbd	800	kg/site-day
Freq: Frequency to Use	Non-default	User-defined	25	days/site-yr
LF: Loss Fraction	Default	Model Parm	0.01	dimensionless
NS: Number of Sites	Default	Mass Parm	1	sites

OK Cancel

View/Update Model Information

Click on the **View/Update Model Information** button in the **Releases** screen to modify the default model parameter values to be used in the calculations.

The **View/Update Release Model Information** screen displays information about the selected model, including: the equation(s) used in the calculation, a description of the basis/source of the model, and a list of the parameters used by the model.

1. To change a parameter value, click on the associated *Type* field.
2. For some parameters, you will change the *Type* field from 'Default' to 'Non-default'. If you choose 'Non-default', you may then click on the associated *Value* field and enter the new value for the parameter (other parameters will prompt you to select from a specified list of alternative values).

❖ In our scenario, the reaction tank is rinsed once every 5 batches, which is $125 \text{ batches} / 5 = 25$ times per year. Therefore, we will change the default frequency of release (Freq) from 125 to 25 days/year.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures

The Releases Tab (continued)

Update release media output specifications

Verify or change the media for the estimated release below. If you are not sure which media is the most appropriate for the estimated release, use the "or" option to designate additional potential media.

Note that when you designate a medium as an "or" case, you can no longer specify a percentage for that medium.

Manufacture of Chemical

Equipment Cleaning Losses of Liquids from a Single, Large Vessel

Basis: EPA/OPPT Single Vessel Residual Model, CEB standard 1% residual

Air:	0 %	<input type="checkbox"/> or Water	<input type="checkbox"/> or Incineration	<input type="checkbox"/> or Landfill
Water:	100 %	<input type="checkbox"/> or Air	<input checked="" type="checkbox"/> or Incineration	<input type="checkbox"/> or Landfill
Incineration:	0 %	<input type="checkbox"/> or Air	<input type="checkbox"/> or Water	<input type="checkbox"/> or Landfill
Landfill:	0 %	<input type="checkbox"/> or Air	<input type="checkbox"/> or Water	<input type="checkbox"/> or Incineration
Other:	0 %			
Destroyed:	0 %			
Total: 100%				

OK Cancel

Modifying the Target Media of Release

Click on the **Modify Media of Release** button in the **Releases** screen to change the default media (i.e., water, air, incineration, landfill) to which the selected source releases will be emitted.

The *Update release media output specifications* screen will appear. In this screen, the selected operation and release source is listed, as well as the selected release model and description of the model basis/source.

In this screen, you can apportion the total amount of the calculated release to more than one target media. Another modification that you may enter in this screen is establishing alternative target media designations.

❖ For example, if the wash water from the reactor vessel rinse (containing residual chemical) may alternatively be incinerated or released to water, the box next to 'or Incineration' that is associated with the 100% release to water is checked.

Run the Models

Click the **Run Model(s)** button in the **Releases** tab to execute the release model calculations.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Releases* Tab (continued)

Case Study - Mock PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Estimating Chemical Releases

All activities that have a chemical release are listed below. Each has one or more release estimation models associated with it. When a release activity is selected, one or more release models will be shown in the Release Model(s) list. Select each model in the Release Model(s) for Selected Activity list to view parameters for the model, and click the View/ Update Model Information button to view model equations and to change parameter values.

Operation: Manufacture of Chemical

Release Activity: Equipment Cleaning Losses of Liquids from a Single, Large Vessel

Release Model(s) for Selected Activity:

- EPA/OPPT Single Vessel Residual Model
- EPA/OPPT Mass Transfer Coefficient Model

Release Input Parameters Estimated Releases

Media	Number of Sites	Daily Release Rate (kg/site-day)	Annual Release Rate (kg/yr-all sites)	Days of Release (days/site-yr)	Basis
Water or Incineration	1	8	200	25	EPA/OPPT

Buttons: Add or Remove a Release model, View/Update Model Information, Modify Media of Release, View/Update Combinations, Run Model(s)

View Release Estimates

Click on the **Estimated Releases** subtab in the **Releases** tab to view the results of the calculations. This screen displays the media of release, the number of sites releasing the chemical, the daily release rate (kg/site-day), the annual release rate (kg/year; all sites), the days of release (days/site-yr), and the basis for the selected release model.

The results for our case study show that 8 kg of chemical per day is released from the manufacturing site over 25 days per year (this is equivalent to 200 kg chemical released per year). The releases are emitted to either water or incineration.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The Releases Tab (continued)

Case Study - Mack PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases Exposures Optional Information

Estimating Chemical Releases

All activities that have a chemical release are listed below. Each has one or more release estimation models associated with it. When a release activity is selected, one or more release models will be shown in the Release Model(s) list. Select each model in the Release Model(s) list for Selected Activity list to view parameters for the model, and click the View/Update Model Information button to view model equations and to change parameter values.

Operation: Manufacture of Chemical

Release Activity: Equipment Cleaning Losses of Liquids from a Single, Large Vessel

Release Model(s) for Selected Activity:

- EPA/OPPT Single Vessel Residual Model
- EPA/OPPT Mass Transfer Coefficient Model

Release Input Parameters Estimated Releases

Media	Number of Sites	Daily Release Rate (kg/site-day)	Annual Release Rate (kg/yr-all sites)	Days of Release (days/site-yr)	Basis
Air	1	0.1139	2.8466	25	EPA/OPPT

Add or Remove a Release model

View/Update Model Information

Modify Media of Release

View/Update Combinations

Run Model(s)

A Source Can Have More Than One Release

In some cases, a source can have associated with it more than one release, and thus more than one release model. In our example, the *Equipment Cleaning Losses of Liquids from a Single, Large Vessel* source used a model that calculated the amount of residual chemical released with the rinse water (i.e., the *EPA/OPPT Single Vessel Residual* model).

The second model shown (the *EPA/OPPT Mass Transfer Coefficient* model) calculates the amount of chemical vapor released to air during the cleaning activity. As previously discussed, this model can also be modified or removed from the assessment.

The amount of fugitive chemical released to air during the reactor vessel cleaning is estimated to be 0.1139 kg chemical per day over 25 days per year (equivalent to 2.8466 kg chemical per year).

View / Update Release Model Information

Read-only and updatable information about the selected release model, including the model equation, mechanism, basis, and input parameters are listed below. Because the release can be calculated using several valid equations for this model, all of the possible parameters that may be used are listed in the Input Parameters grid. Depending on the data values for this release, some of these parameters will not be required. To view options or change a parameter value, click on the label for that parameter under the Type column. When Type is User-defined, you must click on the cell under the value column and type in your own value.

Activity: Equipment Cleaning Losses of Liquids from a Single, Large Vessel

Model: EPA/OPPT Mass Transfer Coefficient Model

Model Equation: DR (kg/site-day) = (G x 3600 x (Dh) / 1000) x (DR occurs over [Freq] days/year)

Mechanism: Volatilization of chemical from "static" pool

Basis: EPA/OPPT Mass Transfer Coefficient Model

Parameter	Type	Value Calc	Value	Units
A: Area	Model Output	Model Param	6647.61	cm ²
d: Diameter of Opening / Pool Length	Default	Model Param	82	cm
Freq: Frequency to Use	Non-default	User-defined	25	days/site-yr
G: Vapor Generation Rate	Model Output	Model Param	0.0316291	g/s
Mw: Molecular Weight	Default	Chem Param	150	daltons
NS: Number of Sites	Default	Mass Param	1	sites

OK Cancel

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Exposures* Tab

Case Study - Mack PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases **Exposures** Optional Information

Estimating Chemical Exposures

All activities that have a chemical exposure are listed below. Each has one or more exposure estimation models associated with it. When an exposure activity is selected, one or more exposure models will be shown in the Exposure Model(s) list. Click on either the Dermal or Inhalation Input Parameters tab below to view parameters for the model, and click the View/Update Model Information button to view model equations and to change parameter values.

Operation: **Manufacture of Chemical**

Exposure Activity: **Loading Liquid Product into Drums**

Dermal Exposure Model: EPA/OPPT 2-Hand Dermal Contact with Liquid Model Liquid

Inhalation Exposure Model: EPA/OPPT Mass Balance Model Vapor

Dermal Model Input Parameters Inhalation Model Input Parameters Activity Exposure Estimates

Parameter	Type	Value Calc	Value	Units
AT: Averaging Time	Default	Model Param	40	years
ATc: Averaging Time over a Lifetime (Chr	Default	Model Param	70	years
BW: Body Weight	Default	Model Param	70	kg
ED: Exposure Days	Default	DDs	125	days/yr
EY: Years of Occupational Exposure	Default	Model Param	40	years
FT: Frequency of Events	Default	Model Param	1	events/site d
NWexp: Number of Workers Exposed	Default	Model Param	3	workers/site
Qs: Quantity for Chemical on Skin, CB	Default	Model Param	2.1	mg/cm2-ever
S: Surface Area	Default	Model Param	840	cm2
Wchem: Weight Fraction of chemical in liq	Default	Ys	0.0	dimensionless

Add or Remove an Exposure model
View/Update Model Information
View/Update Combinations
Run Model(s)

The *Exposures* Tab

Click on the **Exposures** tab to view or modify the models (i.e., algorithms) and associated input parameters used to calculate the inhalation and dermal exposures to workers while performing each of the chosen activities within each of the operations of your assessment. Then click Run Model(s) to generate release estimate results from the model(s).

1. Select an operation from the *Operation* drop down list.
2. Select a source for which exposures are calculated from the *Exposure Activity* drop down list.

❖ The models that are used to calculate the dermal and inhalation exposures from the selected activity within the selected operation appear with the associated form of the chemical.

The parameters used by the dermal and inhalation exposure models appear in the **Dermal Model Input Parameters** subtab and the **Inhalation Model Input Parameters** subtab, respectively. These subtabs also indicate which parameters are ChemSTEER default values, the source of the parameter value (i.e., whether previously input in another tab or calculated from other input parameters), the current value, and the units.

***Note:** ChemSTEER currently contains more than 15 different models that can be used to calculate exposures, each with their own set of default settings and values. You are highly encouraged to review the *ChemSTEER Estimation Methods and Models – Worker Exposures* topic in the **ChemSTEER Help System** for a more complete description of the models and their bases before selecting alternative models to the ChemSTEER defaults and/or modifying default input values.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Exposures* Tab (continued)

Adding or Removing Exposure Models

Click on the **Add or Remove an Exposure Model** button in the **Exposures** screen to change the default models that are used for the selected exposure activity.

The **Add/Remove Exposure Models** screen will appear with drop down lists of alternative dermal and inhalation models that you may choose to use in the assessment.

View / Update Exposure Model Information

Read-only and updatable information about the selected exposure model, including the model equation, mechanism, basis, and input parameters are listed below. Because the exposure can be calculated using several valid equations for this model, all of the possible parameters that may be used are listed in the Input Parameters grid. Depending on the data values for this exposure, some of these parameters will not be required. To view options or change a parameter value, click on the label for that parameter under the Type column. When Type is User-defined, you must click on the cell under the value column and type in your own value.

Activity: Loading Liquid Product into Drums
Model: EPA/DPPT Mass Balance Model

Model Equation: $I = C \times b \times h$
 $LADO = (I \times ED \times Y) / (BW \times ATc \times 365 \text{ days/yr})$

Mechanism: Inhalation of chemical vapors

Chemical State: Vapor

Basis: EPA/DPPT Mass Balance Model

Parameter	Type	Value Calc	Value	Units
EY: Years of Occupational Exposure	Default	Model Param	40	years
G: Vapor Generation Rate	Model Output	Model Param	0	g/s
h: Exposure Duration	Non-default	User-defined	2	hrs/day
I: Mixing Factor	Default	Model Param	0.1	dimensionless
MW: Molecular Weight	Default	Chem Param	150	daltons
Nw/wn: Number of Workers Exposed	Default	Model Param	3	workers/site

OK Cancel

View/Update Model Information

Click on either the **Dermal Model Input Parameters** or the **Inhalation Model Input Parameters** subtab and click the **View/Update Model Information** button in the **Exposures** screen to modify the default model parameter values to be used in the calculations.

The **View/Update Exposure Model Information** screen displays information about the selected model, including: the equation(s) used in the calculation, a description of the mechanism of exposure, the chemical state, the basis/source of the model, and a list of the parameters used by the model.

1. To change a parameter value, click on the associated *Type* field.
2. For some parameters, you will change the *Type* field from 'Default' to 'Non-default'. If you choose 'Non-default', you may then click on the associated *Value* field and enter the new value for the parameter (other parameters will prompt you to select from a specified list of alternative values).

❖ In our scenario, we previously found that drums are filled for approximately 2 hours per day (see *Entering Container Parameters*). Therefore, we may change the default exposure duration (h) from the default of 8 to 2 hours/day.

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Exposures* Tab (continued)

Case Study - Mack PMN

File Edit Reports Help

General Chemical Operations Operation Parameters Releases **Exposures** Optional Information

Estimating Chemical Exposures

All activities that have a chemical exposure are listed below. Each has one or more exposure estimation models associated with it. When an exposure activity is selected, one or more exposure models will be shown in the Exposure Model(s) list. Click on either the Dermal or Inhalation Input Parameters tab below to view parameters for the model, and click the View/Update Model Information button to view model equations and to change parameter values.

Operation:

Exposure Activity:

Dermal Exposure Model: EPA/OPPT 2-Hand Dermal Contact with Liquid Model Liquid

Inhalation Exposure Model: EPA/OPPT Mass Balance Model Vapor

Dermal Model Input Parameters Inhalation Model Input Parameters **Activity Exposure Estimates**

Exposure	Estimate	Units
Inhalation Potential Dose Rate	140.69	mg/day
Inhalation Lifetime Average Daily Dose	0.3933	mg/kg-day
Inhalation Average Daily Dose	0.6893	mg/kg-day
Inhalation Acute Potential Dose	2.0099	mg/kg-day
Dermal Exposure Dose Rate	1,411.2	mg/day
Dermal Lifetime Average Daily Dose	3.9452	mg/kg-day
Dermal Average Daily Dose	6.9041	mg/kg-day
Dermal Acute Potential Dose	20.16	mg/kg-day

Add or Remove an Exposure model

View/Update Model Information

View/Update Combinations

Run Model(s)

Run the Models

Click the **Run Model(s)** button in the **Exposures** tab to execute the exposure model calculations.

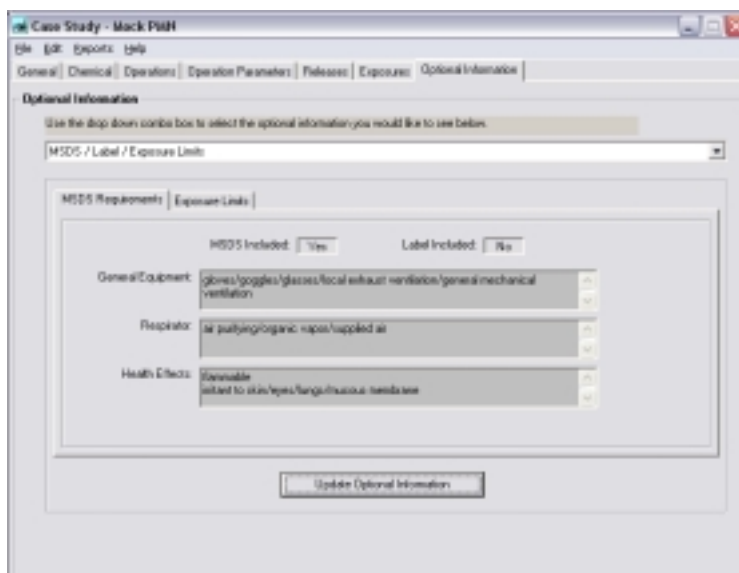
View Exposure Estimates

Click on the **Activity Exposure Estimates** subtab to view the results of the calculations. This screen displays the type of exposure, the estimated value, and the associated units.

The results for our case study show that the workers may inhale approximately 141 mg of chemical vapors per day during drum filling activities. In addition, they come into contact with 1,411 mg of the liquid chemical on their hands daily during the filling activity. These values are potential dose rates.

The inhalation and exposure models also calculate several other types of dose rates: lifetime average daily dose, average daily dose, and acute potential dose (all in units of mg/kg-day).

Case Study Utilizing ChemSTEER – Workplace Releases and Exposures The *Optional Information* Tab



The *Optional Information* Tab

To enter additional information about your assessment, click on the ***Optional Information*** tab.

This tab contains several input screens that you may select from the drop down list, including:

- ❖ MSDS/Label/Exposure Limits
- ❖ Pollution Prevention Considerations
- ❖ General assumptions used in the assessment

Some of the input screens are designed to serve EPA-related assessments and may be left incomplete, including:

- ❖ SAT Data
- ❖ Exposure-based Criteria
- ❖ Other Uses, Occupational Exposure Rating, and Consumer Use.

Saving and Opening Your Assessments

You can save assessments as individual records in a database file containing multiple records or as their own individual database files using File/ Save or /Save As options on the Menu Bar.

If you open an Assessment (record) from an existing database file, you may view and/or edit the assessment on the ChemSTEER interfaces (screen views).

You may choose File/ Save Assessment to overwrite the Assessment that is in the existing database file with the working assessment that is displayed on the ChemSTEER interfaces.

If the existing database file contains more than one Assessment record, a table of Assessment records will appear that includes four fields in the record: Type, Identifier, Status, and Date. These fields must be completed on the General screen (the first screen that appears after running ChemSTEER).

You should review the ChemSTEER Help topics under the Guide to ChemSTEER Menus (File) to learn more about saving and opening assessments.